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ABSTRACTS

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Plenary session

PL-1

CONNECTIVITY BETWEEN STRUCTURE AND DYNAMICS IN GLASS-FORMING LIQUIDS

Limei Xu
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The structural description for the link between the fast vibrational dynamics and slow diffusive dynamics in glass-forming systems is one of the most challenging issues in physical science. In this talk, I will discuss structural origin and its correlation with dynamic transition in supercooled liquids. Particular, in a model of metallic supercooled liquid, we find that local connectivity as an atomic-level structural order parameter tunes the short-time vibrational excitations of the icosahedrally coordinated particles and meanwhile modulates their long-time relaxation dynamics changing from stretched to compressed exponentials, denoting a dynamic transition from diffusive to hyperdiffusive motions. Our result indicates that long-time dynamics has a structural origin, thus suggesting a structural link the fast vibrational dynamics and the slow structural relaxation in glassy materials.

PL-2

DYNAMIC BEHAVIOR AND DIRECTED ORGANIZED ASSEMBLY OF BIOPOLYMER COMPONENTS IN ANISOTROPIC PHASES AND SOLID STATE

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We discuss recent results from our research group on designing soft and strong responsive polymer and biopolymer nanocomposite materials and structures for sensing and bio-derived photonic nanomaterials as summarized in our recent reviews [1, 2]. Ultrathin silk fibroin proteins and cellulose nanocrystals/nanofibers are combined with functionalized graphene oxide sheets for prospective applications functional nanocomposites. In first approach, we fabricated uniformly aligned chiral photonic bioderived films from a liquid crystal phase formed by a cellulose nanocrystal solution placed in a thin capillary [3]. This confinement facilitates a slow homogeneous growth of chiral pseudo-layers parallel to the interface in contrast to the highly heterogeneous process of drying from the drop-cast approach. The preferential evaporation of water along the air/water interface induces a saturated vapor promoting unidirectional propagation of the ordered phase in large regions that results in chiral CNC solid films with uniformly oriented layered morphology. The resulting films show a much narrower optical reflectance band and uniform birefringence over larger macroscopic regions than highly heterogeneous conventional drop-cast films. These thin films with controllable and well-identified structural colors and handiness open up interesting possibilities for broad applications in flexible biophotonics. In another related study, we observed that combining of biological components such as silks and cellulose nanofibers can result in formation of peculiar 1D shish-kebab nanostructures for functional porous robust membranes [4].

References

[1] R. Xiong, A. M. Grant, R. Ma, S. Zhang, V. V. Tsukruk, Naturally-derived polymers and bionanocomposites, *Mat. Sci.&Eng. Reports*, 2018, in print
[2] S. Zhang, R. Geryak, J. Geldmeier, S. Kim, V. V Tsukruk,' Synthesis, assembly, and applications of hybrid nanostructures for biosensing, *Chem. Rev.* **117**, 12942 (2017)
[3] V. Cherpak, V.F. Korolovych, T. Turiv, D. Nepal, J. Kelly, T.J. Bunning, O.D. Lavrentovich, V.V. Tsukruk, Uniform Chiral Organization of Cellulose Nanocrystals in Capillary Confinement, 2018, submitted
[4] R. Xiong, H. S. Kim, S. Zhang, S. Kim, V. F. Korolovych, R. Ma, Y. Yingling, C. Lu, V. V. Tsukruk, Template-Guided Assembly of Silk Fibroin on Cellulose Nanofibers for Robust Nanostructures with Ultrafast Water Transport, *ACS Nano,* **11**, 12008-12019 (2017).

PL-3

HYDRODYNAMIC TURBULENCE OF SUPERfluIDS HELIUM: BASIC IDEAS, EXPERIMENTS AND PHYSICAL MODEL

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Liquid ^{4}He and ^{3}He at very low temperature become a quantum fluid, consisting of interacting viscous normal and inviscid superfluid components with quantized vortex lines. It is tempting to think that the statistical properties of such a complex fluid are very different from the classical fluids. That is not necessarily so, the turbulence of classical and quantum fluids have much in common, although the differences sometimes are very important.
I will remind basic ideas in turbulence of classical fluids, the peculiarities of superfluid dynamics and turbulence and discuss the recent ideas, experiments and physical models of superfluid turbulence.

PL-4

SUPRAMOLECULAR POLYMERS AS RESPONSIVE FUNCTIONAL MATERIALS

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The constitutional and conformational dynamics related to supramolecular polymers has recently opened a series of very intriguing possibilities in chemical science.[1] For instance, within this framework, emerging lines of investigations have been directed towards the development of dynamic materials and devices.[2] These ones can be defined as multi-component chemical systems which, thanks to the reversibility of their interconnections and to their sensitivity to environmental parameters, aim at performing modular functional tasks by responding to external stimuli. The behavior of such dynamic materials is by essence more complex than the one produced by their static or single-component counterparts and as such, they hold higher potentialities in terms of information processing and functionality tuning. We will discuss some of our works concerning such responsive systems along these lines and, more particularly, we will focus on highly conducting supramolecular polymers[3] and on out-of-equilibrium polymer / molecular motor conjugates.[4]

References

(a) Moulin, E., Giuseppone, N. – Encyclopedia of Supramolecular Chemistry – From molecules to nanomaterials - Reactions in Dynamic Assemblies, John Wiley & Sons, Ltd**., 4,** 1543 (2012); (b) Giuseppone, N., *Acc. Chem. Res.*, **45**, 2178 (2012).
(a) Moulin, E., Cormos, G., Giuseppone, N., *Chem. Soc. Rev*. **41**, 1031 (2012); (b) Busseron, E., Ruff, Y., Moulin, E., Giuseppone, N., *Nanoscale*, **5**, 7098 (2013).
(a) E. Moulin, F. F. Niess, M. Maaloum, E. Buhler, I. Nyrkova and N. Giuseppone, *Angew. Chem. Int. Ed*. **49**, 6974 (2010); (b) V. Faramarzi, F. Niess, E. Moulin, M. Maaloum, J.-F. Dayen, J.-B. Beaufrand, S. Zanettini, B. Doudin and N. Giuseppone, *Nature Chem.*, **4**, 485 (2012); (c) E. Moulin, J.-J. Cid and N. Giuseppone, *Adv. Mater.*, **25**, 477 (2013); (d) J. J. Armao, M. Maaloum, T. Ellis, G. Fuks, M. Rawiso, E. Moulin and N. Giuseppone, *J. Am. Chem. Soc.*, **136**, 11382 (2014); (e) J. J. Armao, P. Rabu, E. Moulin and N. Giuseppone, *Nano Lett.*, **16**, 2800 (2016); (f) J. J. Armao IV, I. Nyrkova, G. Fuks, A. Osypenko, M. Maaloum, E. Moulin, R. Arenal, O. Gavat, A. Semenov, N. Giuseppone, *J. Am. Chem. Soc.*, **139**, 2345 (2017).
(a) G. Du, E. Moulin, N. Jouault, E. Buhler, N. Giuseppone, *Angew. Chem. Int. Ed.*, **51**, 12504 (2012); (b) Goujon, A., Du, G., Moulin, E., Fuks, G., Maaloum, M., Buhler, E., Giuseppone, N., *Angew. Chem. Int. Ed.*, **55**, 703 (2016**)**; (c) Li, Q., Fuks, G., Moulin, E., Maaloum, M., Rawiso, M., Kulic, I., Foy, J. T., Giuseppone, N., *Nature Nanotech.*, **10**, 161 (2015**)**; (d) Foy, J., Li, Q., Goujon, A., Colard-Otté, J.-R., Fuks, G., Moulin, E., Schiffmann, O., Dattler, D., Funeriu, D. P., Giuseppone, N., *Nature Nanotech.*, **12**, 540 (2017).

PL-5

NOVEL MEDICAL AND BIOTECHNOLOGICAL APPLICATIONS OF MAGNETIC FLUIDS

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Magnetic fluids or ferrofluids are stable colloidal suspension of magnetic nanoparticles in a carrier liquid that can be aqueous or oil-based. Magnetic nanoparticles have generated considerable research and commercial interest due to their unique properties and wide applicability. The unique properties include susceptibility to external magnetic field and biocompatibility. We have developed a number of technologies specifically with bare magnetic nanoparticles which are technically proficient and industrially viable. Most of the applications till date use surface modified/coated magnetic nanoparticles. On the contrary, our applications use bare/uncoated magnetic nanoparticles that are cost effective, simpler to make and use.

Magnetic nanoparticles can be conjugated with drugs and injected intravenously. Further by the use of an external magnetic field they can be transported and retained at the site of action like cancerous tumor or arterial blockage. Some recent developments have also shown a potent approach for delivery of a gene or small interfering RNA (siRNA) using magnetic nanoparticles. Delivering a gene/si-RNA without any carrier makes it prone to rapid degradation by exonucleases or endonucleases and poor diffusion across the cell membrane. We are developing an oligonucleotide-Magnetic Nanoparticle (Oligo-MNP) complex in order to overcome these problems. Magnetic hyperthermia is another promising application wherein providing an external alternating magnetic field to nanosized magnetic particles causes heating via hysteresis energy losses. This approach can be used to kill cancerous cells in the body. Studies have also demonstrated the use of magnetic nanoparticles to improve MRI (magnetic resonance imaging) contrast. This MRI contrast enhancement relies on the differential engulfment of magnetic nanoparticles by different cells.

Our current research is based on the development of methods wherein magnetic nanoparticles are used for a rapid, efficient and contamination-free extraction of biomolecules like DNA, RNA and proteins. These technologies will be helpful to various research labs and industries in minimizing their efforts to isolate specific biomolecules. In this regard XpressDNATM kits are already in the market for rapid DNA isolation from various biological samples. Another exciting prospect is the immobilization of proteins on magnetic nanoparticles for specific applications. Enzymes immobilized on magnetic nanoparticles were found to be active for “several days” in harsh conditions. This application can potentially change the way enzymes are used in industries. Immobilization of antibodies on magnetic nanoparticles on the other hand can be efficiently used for isolation of rare cells, immune cells or cancer cells from blood or a variety of tissues. These strategies have been proven to be highly usable at laboratory scale. We are looking forward to develop these technologies and bring them to the market to benefit the existing research and the industrial setups. Most importantly we are developing an instrument for purification of therapeutic proteins using our patented technology wherein affinity ligands immobilized on the surface of magnetic nanoparticles will enable rapid purification of therapeutic proteins like antibodies.

PL-6

SELF-ORGANIZATION AND STRUCTURAL TRANSITIONS IN SHAPE-ANISOTROPIC COLLOIDS

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In last decades, the self-organisation in colloids with highly anisotropic particles (carbon nanotubes, platelets of grapheme and laponite and their mixtures), attract great attention. Different hosts (simple liquids, liquid crystals and soft polymers) were tested for making these metamaterials with attractive electrophysical, optical and mechanical properties, electro-optical memory effects, and ultra-low percolation thresholds. This report reviews the problems of dispersion of highly anisotropic particles in different host media. Examples of electro-physical, rheological and percolation behaviour in these systems are extensively reviewed. Special attention is paid to Monte Carlo simulations with examples self-organization and structural transitions driven by Brownian motion and drying of colloidal suspensions. Data on impact of particle aggregation on optical properties and application of the Beer-Lambert law to optically anisotropic colloids are also presented.

A TWO-STATE PICTURE OF WATER AND THE FUNNEL OF LIFE

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Abstract: I will discuss recent experimental and simulation data of liquid water and the picture of fluctuations between high-density (HDL) and low-density (LDL) liquid this has led to [1,2]. The HDL would be a more close-packed form, favored by entropy and dominates at high temperature. Below about 50°C correlated fluctuations into tetrahedral (LDL) structures, favored by hydrogen-bonding (enthalpy), begin to appear and become increasingly important upon further cooling [3,4]. A coexistence line between the two liquid phases is hypothesized, but it must lie at high pressure and low temperature in the so-called "No-man's land" where measurements are extremely challenging due to rapid crystallization [5,6]. If such a line exists, it may terminate in a critical point from which a funnel-like region of enhanced fluctuations between the two forms emanates. Indeed, in a very recent study the isothermal compressibility and correlation length were measured down to 227 K and shown to exhibit a maximum which can be viewed as a trace of a critical point[7]. Since these fluctuations are observed up to ambient conditions we may live in what could be called the "funnel of Life". In light of this picture I will discuss some of the more important anomalous properties of water.

References:

[1] Anders Nilsson and Lars G.M. Pettersson, *The Structural Origin of Anomalous Properties of Liquid Water*, Nature Commun. **6**, 8998 (2015).
[2] P. Gallo *et al*., *Water: A Tale of Two Liquids*, Chem. Rev. **116**, 7463-7500 (2016).
[3] L. B. Skinner *et al*., *The Structure of Water Around the Compressibility Minimum*, J. Chem. Phys. **141**, 214507 (2014).
[4] D. Schlesinger, K.T. Wikfeldt, L.B. Skinner, C.J. Benmore, A. Nilsson and L.G.M. Pettersson, *The temperature dependence of intermediate range oxygen-oxygen correlations in liquid water*, J. Chem. Phys. **145**, 084503 (2016).
[5] J. A. Sellberg *et al*., *Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature*, Nature **510**, 381 (2014)
[6] F. Perakis *et al*., *Diffusive dynamics during the high- to low-density transition in amorphous ices*, Proc. Natl. Acad. Sci. **114**, 8193 (2017)
[7] Kim, K.-H. *et al. Maxima in the Thermodynamic Response and Correlation Functions of Deeply Supercooled Water*, Science **358**, 1589 (2017)

CRITICAL AND NON-CRITICAL FLUCTUATIONS IN MIXTURES OF IONIC LIQUIDS WITH ALCOHOLS IN THE VICINITY OF THE LIQUID-LIQUID PHASE TRANSITION

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Mesoscopic heterogeneities in binary mixtures of the ionic liquid ethyl-ammonium nitrate (EAN) with alcohols (pentanol and heptanol) are investigated by Small Angle X-ray Scattering as function of concentration and temperature ranging from 193 to 313 K. Such systems in general show a liquid-liquid phase transition which is driven by Coulomb interactions but modified by hydrogen bonding. Though macroscopically homogeneous, the mixtures are heterogeneous at the mesoscopic spatial scales. Two different heterogeneities are present: Critical concentration fluctuations centred at scattering vector Q=0, well known as precursors of the liquid-liquid phase transition e.g. for EAN/Octanol mixtures [1], and heterogeneities caused by segregation into ionic and non-ionic regions. The latter ones were predicted by simulation [2] and verified experimentally [3] in ionic liquids containing cations with long hydrocarbon chains. In pure EAN such structuring is observed as well giving rise to a band centred near Q = 6 nm-1 [4]. A similar band at Q =5 nm-1 is also observed in alcohols, again suggesting a segregation into polar and no-polar regions as a special case of charge ordering. Those heterogeneity bands of EAN and alcohols merge in mixtures. When approaching the critical composition and lowering the temperature towards the critical temperature, critical concentration fluctuations dominate and overshadow the ionic-non-ionic heterogeneity band. A careful analysis shows that this band reveals but is shifted towards small figures of the scattering vector. The Q=0 band varies with concentration, temperature and Q as expected for critical fluctuations. For the system EAN / heptanol the phase diagram was measured with an upper critical solution point at 259K and a critical composition at x= 0,64. In the case of the pentanol system [5] the critical solution point is virtual as it lays inside the solid phase region and thus cannot be reached in the experiment. For this system the critical temperature is estimated by extrapolation to Tc≈190 K. A pseudo spinodal is constructed applying the scaling laws of critical fluctuations.

References

[1] W. Schröer, S. Wiegand, H. Weingärtner, Ber. Bunsen. Ges. Phys. Chem. **97**, 975 (1993)
[2] J.N.Canongia Lopes, A.A.H Padua, J. Phys. Chem. B. **110**, 3330 (2006)
[3] A. Triolo, O. Russino, H.J. Bleif, E.Di Cola, J Phys, Chem. B **111**, 4641(2007)
[4] R. Hayes, S. Imberti , G. G. Warr, R. Atkin, PCCP **13**, 3237 (2011)
[5] W Schroer, A Triolo, O Russina, J. Phys. Chem. B **120**, 2638 (2016)

PL-9

THE WAY TO FIGHT WITH THE AMYLOID PROTEIN AGGREGATES: ROLE OF NANOPARTICLES

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Abnormal protein aggregation and accumulation of formed fibrils are characteristic features for a range of, if not all, neurodegenerative disorders such as Alzheimer's, Huntington's, Parkinson's, as well as non-neuropathic amyloidosis. Amyloid fibrils-related pathologies are still incurable diseases. Nevertheless, inhibition and/or reduction of amyloid aggregates is considered as the primary therapeutic strategy [1,2]. Nanoparticles (NPs), due to their size-dependent physical and chemical properties, have shown remarkable potential for a wide range of applications over the past decades. For example, NPs are being explored for their role in diagnosing, preventing, treating or even causing amyloid diseases. Thus, it was demonstrated that NPs can significantly influence the process of protein amyloid fibrillization. In addition to amyloid pathology, our aim was to study the physical properties of the bio-nano-composites, particularly those, which contain within themselves magnetic (Fe_3O_4-based) nanoparticles. The results demonstrated that magnetic component of magnetic fluids was important for their anti-amyloid activity, however, the physico-chemical properties of NPs such as type of coating layer, charge, concentration, etc. determined the extent of inhibition/depolymerization activity [3-5]. Recently we have tested the ability of irradiation to enhance the effect of (Fe_3O_4-based) NPs and the effect of cerium oxide nanoparticles on amyloid fibril formation.

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References:

[1] De Felice, F. G., Ferreira, S.T. *Cell. Mol. Neurobiol.*, **22**, 545−563 (2002).
[2] Khlistunova, I., Biernat, J., Wang, Y. et al. *J. Biol. Chem.* **281**, 1205−1214 (2006).
[3] Bellova, A., Bystrenova, E., Koneracka, M., et al. *Nanotechnology*, **21(6)**, 065103 (2010).
[4] Siposova K., Kubovcikova, M., Bednarikova Z. et al. *Nanotechnology*, **23(5)**, 055101 (2012).
[5] Siposova, K., Pospiskova, K., Bednarikova, Z., et al. *JMMM*, **427**, 48−53 (2017).

PL-10

APPLICATIONS OF FLUCTUATING HYDRODYNAMICS TO NON-EQUILIBRIUM STEADY STATES

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Fluctuating Hydrodynamics (FHD) is a mesoscopic extension of classical hydrodynamics, jointly invented in the former Soviet Union by Nobel prize winner Lev Landau and the Ukrainian physicist Evgeny Lifshitz [1]. Well publicized through their famous Course of Theoretical Physics [2], the basic idea behind FHD is as follows: In hydrodynamics the balance equations (mass, momentum, energy,...) need to be complemented with (linear) phenomenological laws which relate the so-called dissipative fluxes with the gradients of thermo-hydrodynamic fields. Landau and Lifshitz [1-2] proposed that, to reflect the stochastic nature of the atomic interactions responsible of dissipation, the linear laws should be considered to be valid only 'on average', needing to be supplemented with random dissipative fluxes. To fix ideas one can consider, for instance, the case of a diffusion flow $\boldsymbol{J}$ in an isothermal binary fluid mixture (Fick's law) for which FHD proposes an stochastic phenomenological law, namely

$$\boldsymbol{J} = -\rho D \nabla c + \delta \boldsymbol{J} \qquad (1)$$

where ρ, D and ∇c are the mass density, the diffusion coefficient and the concentration gradient (in mass fraction), respectively. Most importantly, $\delta \boldsymbol{J}$ in eq. (1) represents a random diffusion flow. To recover the classical Fick's law on average, one must have $\langle \delta \boldsymbol{J} \rangle = 0$. Substitution of expressions like (1) into the balance laws (balance of mass for this particular case) transforms the hydrodynamic equations into a set of partial **stochastic** differential equations. By averaging (over fluctuations) one re-obtains the classical or **deterministic** equations. But the stochastic FHD equations make it possible to discuss the physical nature of spontaneous thermal fluctuations, and evaluate explicit expressions for their time correlation functions. However, to proceed in that direction one needs to know the statistical properties of $\delta \boldsymbol{J}$, beyond the cancellation of the first moment. The contribution of Landau and Lifshitz [1-2] is to realize that, since for **global equilibrium** states natural or spontaneous fluctuations in the thermodynamic variables (density, number of particles, etc.) are known from Statistical Physics (canonical ensemble), the second moment of the random dissipative fluxes must be given by the so-called Fluctuation-Dissipation Theorem (FDT). In the particular case of eq. (1) the FDT means that the components of the random diffusion flux for an isotropic fluid are correlated as:

$$\left\langle \delta J_i(\boldsymbol{r},t) \cdot \delta J_i(\boldsymbol{r}',t') \right\rangle = 2 k_{\mathrm{B}} T \, \rho D \left(\frac{\partial c}{\partial \mu} \right)_{T,p} \delta_{ij} \; \delta(\boldsymbol{r}-\boldsymbol{r}') \; \delta(t-t') \qquad (2)$$

In eq. (2) k_{B} is Boltzmann's constant, T is the temperature (uniform for a global equilibrium state) and $\left(\partial c / \partial \mu\right)_{T,p}$ the osmotic compressibility (the **thermodynamic factor** in the theory of diffusion). In addition, $\boldsymbol{r}$, $\boldsymbol{r}'$ are two position vectors and t, t' two values of time. In principle, the FDT (2) is only rigorously valid for fluctuations in a global equilibrium state [3,4], in which case statistical physics provides a justification.

In my presentation I shall review work performed in the last two decades, which extended Landau-Lifshitz FHD for the evaluation of spontaneous thermal fluctuations around non-equilibrium (NEFs) steady states [3]. This work implied the adoption of a local equilibrium version of the FDT (2). It turns out that mode-coupling phenomena that do not exists in equilibrium, causes in many instances the NEFs to be strongly enhanced. Moreover, opposite to equilibrium ones, equal-time NEFs have, generically, a long spatial range. The combination of these two characteristics lead these NEFs to be referred to as **Giant Fluctuations**. In addition, the generic long-spatial-range causes the presence of boundaries (walls) to strongly affect the NEFs spatio-temporal spectrum, including the recently predicted appearance of NEFS-induced **Casimir forces** [4]. I also shall briefly review experimental confirmation of several features of NEFs, including planned space experiments [5].

References

[1] L. D. Landau, E. M. Lifshitz, Hydrodynamic Fluctuations, Sov. Phys. JETP, 5, 1957, p. 512-513. Zh. Eksp. Teor. Fiz., **32**, 618 (1957).
[2] L.D. Landau, E.M. Lifshitz, Fluid Mechanics, Pergamon, London, 1959.
[3] Ortiz de Zárate, Sengers. Hydrodynamic Fluctuations in Fluids and Fluid Mixtures. Elsevier, Amsterdam, 2006
[4] T.R. Kirkpatrick, J.M. Ortiz de Zárate, J.V. Sengers. Giant Casimir effect in fluids in nonequilibrium steady states. Phys. Rev. Lett., **110**, 235902 (2013).
[5] Baaske, Bataller, Braibanti, Carpineti, Cerbino, Croccolo, Donev, Köhler, Ortiz de Zárate, Vailati. The NEUF-DIX space project. Non-EquilibriUm Fluctuations during DIffusion in compleX liquids. Eur. Phys. J. E **39**, 119 (2016).

COMMAND OF SWIMMING BACTERIA BY ANISOTROPIC LIQUIDS

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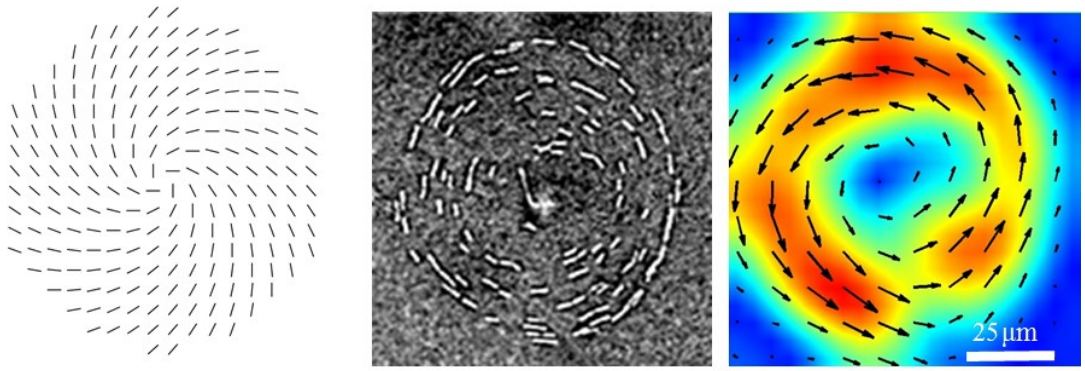
Self-propelled bacteria are marvels of nature. If we can control their dynamics, we could use it to power microsystems of the future. Unfortunately, bacteria swim mostly randomly in isotropic liquids such as water. It is difficult to control them by factors other than transient gradients of nutrients; visual, acoustic and tactile communication channels that humans use to control large animals are not effective. To establish communication, we replace water with a water-based anisotropic liquid, the so-called lyotropic liquid crystal, which couples propulsion of bacteria to the orientational order of the medium. The anisotropy axis can be designed as uniform or be pre-patterned into various structures by a plasmonic photoalignment technique [1]. The preimposed patterns of molecular orientation allow one to gain a significant control over the dynamics of bacteria, namely, their trajectories, polarity of swimming, spatial variation of concentration [2], and run-and-tumble behavior [3]. Topological defects of integer strength serve either as attractors or repellents of bacteria, while defect pairs and patterns with broken left-right symmetry pump the bacterial flows along a preselected polar axis. The patterns can be designed to force a unipolar swimming of bacteria, as shown in the figure [2]. The systrem offers an unprecedented opportunity to test the modern theories of active matter. The study of bacteria-liquid crystal system might result in approaches to harness the energy of collective motion for micro-robotic, biomechanical, and sensing devices, as well as micro-mixing and transport of micro-cargo. The work is supported by US NSF grants DMR-1507637 and DMS-1729509.



Unidirectional circulation of swimming bacteria around the core of a topological defect in a liquid crystal; left: director field; center: swimming bacteria; right: velocity field.

References

[1] C. Peng, Y. Guo, T. Turiv, M. Jiang, Q.-H. Wei, O.D. Lavrentovich, Advanced Materials **2017**, 1606112 (2017).
[2] C. Peng, T. Turiv, Y. Guo, Q.-H. Wei, O.D. Lavrentovich, Science **354**, 882 (2016).
[3] S. Zhou, O. Tovkach, D. Golovaty, A. Sokolov, I.S. Aranson, O.D. Lavrentovich, New Journal of Physics **19**, 055006 (2017).

PL-12

VIBRATIONAL SPECTROSCOPY APPLIED TO SOLUTION AND METAL/SOLUTION INTERFACE CHEMISTRY STUDIES

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Important results for the biology and industrial areas are here presented. For the former, our group has often employed Raman and IR spectroscopies to build spectral patterns for systems containing simple protic amides and metal ions [1], and the goal is to better understand why only certain metals cleave the peptide bond. So far, we have observed that the kind of metal significantly changes the amide spectrum. That is, the ν_{CO} mode (1700 cm^{-1}) is upshifted as high electrostatic potential (φ) metal ions are added, but the replacement for ions containing φ values varying from moderate to low leads to the upshift of the ν_{CN} vibration (1310 cm^{-1}). Most recently, the γ_{HNH} mode (1190 cm^{-1}), which is inactive in both techniques, is activated only in the IR spectrum as ions with high φ values are present (Figure 1).

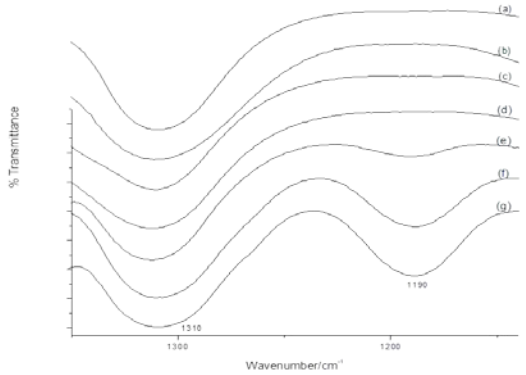

Figure 1. Infrared spectra of liquid formamide and its solutions containing various metal ions: (a) solvent; (b) Zn(II); (c) Ni(II); (d) Co(II); (e) Al(III); (f) Ga(III); (g) Zr(IV).

The importance in the development of new corrosion inhibitors for the industry is out of discussion, even though some fundamental aspects related to their action mode remain unanswered. Our SERS results [2] show for the first time that the imidazole:imidazolium couple is adsorbed on the copper surface not only at acidic pH, but also at basic one. The neutral molecule changes the orientation from tilted to perpendicular as the potential is made more negative, while the cation remains parallel for the whole studied potential range. A chemisorption mechanism is proposed at more cathodic potentials, but it changes to physisorption near the copper corrosion potential (E = -0.07 V) and finally a reaction between the inhibitor and the oxidized metal surface takes place at more anodic potentials (Figure 2).

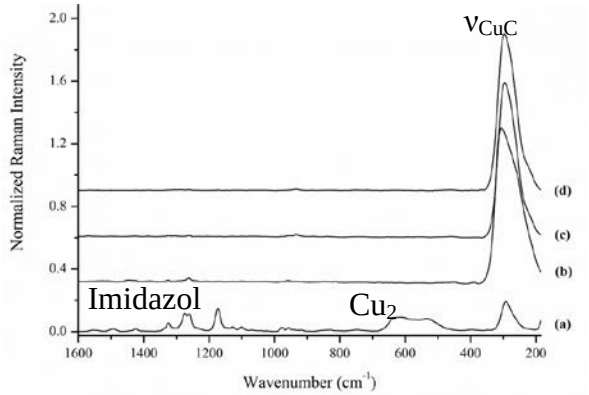

Figure 2. SERS spectra from a diluted imidazole solution at different E (V): (a) -0.07; (b) 0.0; (c) 0.2; (d) 0.4.

References

[1] A. K. M. S. Gomes and W. A. Alves, *Vib. Spec.*, **89**, 57-61 (2017).
[2] E. F. Silva, M. C. E. Bandeira, W. A. Alves and O. R. Mattos, *J. Electrochem. Soc.*, (2018) in press.

PL-13

HEAVY ION INDUCED DNA STRUCTURE CHANGES IN A LIQUID ENVIRONMENT

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The structure of DNA is essential in maintenance and alteration of biological inherited characters. The effects of ionizing radiation result from the deposition of energy in the cell nucleus producing damage to the DNA target and that the consequences of the damage are expressed in the irradiated cell. To understand these features, we need to obtain detailed knowledge of interactions between beams and DNA in a liquid environment. In this talk, I will present recent progress made on the DNA conformational changes induced by heavy ion.

PL-14

MD-MODELING OF THE INTERMEDIATE SCATTERING FUNCTION FOR ARGON-LIKE LIQUIDS AND WATER

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The spectral densities of the intermediate scattering function (ISF) for argon-like liquids and water are studied with the help of computer simulations. Note, that in the case of water only translational motions for the centers of mass of molecules are taken into account. The applicability region of the diffusion approximation for the ISF, $0 \le |\vec{k}| < k_D(T),\ 0 \le \omega < \omega_D(\vec{k},T)$, is investigated. It is shown that the upper limit $k_D(T)$ for wave vectors $\vec{k}$ depends on temperature and satisfies the inequality: $k_D(T) << 1/a$, where a is the interparticle spacing. Analogously, the upper limit $\omega_D(\vec{k},T)$ for frequencies depends on wave vector and temperature and it is surprisingly small: $\omega_D(\vec{k},T) \sim \gamma_D(\vec{k}^2)$, where $\gamma_D(\vec{k}^2)$ is the half-width for the Lorentzian: $\gamma_D(\vec{k}^2) \sim D_s\vec{k}^2$, and D_s is the self-diffusion coefficient. Non-analytical contributions to the half-width of the ISF spectral density are discussed. It is shown that the leading term of the non-analytical contributions is proportional to the ratio: D_c / D_s, where D_c is the collective part of the self-diffusion coefficient. The comparative behavior of $\gamma_D(\vec{k}^2)$ as functions of wave vectors for water and argon is discussed. The role of rotational contributions to the ISF is discussed. It had been shown that main peculiarities of the ISF-spectra are determined by translational motion of water molecules.

#SECTION_0_POSTERS#

Section 1. Water, Water Systems.

Oral session

1-1.O

HYPERTHERMIA EFFECT IN VARIOUS IRON OXIDES

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Magnetic nanoparticles are key components for development of many novel bio- and nanotechnological applications. The existence of biocompatible phospholipid membrane around magnetosome and the high value of specific absorption rate (*SAR)* about $900 W \cdot g^{-1}$ predetermine this bacterial nanoparticles for the biomedical applications. Usually the magnetosome are prepared by biomineralization process of magnetotactic bacteria *Magnetospirillum sp.AMB-1.*The magnetosome chains were divergent in length i.e. chains of magnetosomes have been modified due to mechanical effects during sonication. In this contribution we present the influence length of chains on the hyperthermia effect and magnetosome chains characterization via small-angles techniques [1].
On the other hand magnetoferritin is a synthetic derivate of ferritin, an iron storage protein. It is composed of apoferritin shell and iron-based magnetic nanoparticles, providing higher sensitivity to an applied magnetic field allowed to study hyperthermic effect in magnetoferritin aqueous colloidal solution. Here we are presenting the first results from measurement a temperature increase versus time for various intensities of magnetic fields. Specific Absorption Rate (SAR) values for various magnetic field intensity were in the range 3.2 – 5.0 $W.g^{-1}$. The low hyperthermic effect of magnetoferritin could be related to small sizes of magnetoferritin cores, which polyphase structure was largely composed of lepidocrocite-like mineral.

References

[1] M. Molcan, H. Gojzewski, A. Skumiel, S. Dutz, J. Kovac, M. Kubovcikova, Timko, M.: *Journal of Physics D-Applied Physics*, **49(36)** (2016)
[2] L. Balejcikova, V.M. Garamus, M.V. Avdeev, V.I. Petrenko, L. Almásy, P. Kopcansky: *Coll. and Surf.B: Biointerfaces* **156**, 375–381 (2017).

THE DISTINCT PROPERTIES OF A WATER ELECTRODE IN CONTACT WITH AN AC POWERED DIELECTRIC BARRIER MICRO-DISCHARGE

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Although plasmas in contact with liquids have recently gained increasing interest due to their various promising applications in medicine, agriculture and water treatment, the fundamental features of a liquid electrode are still largely unexplored [1]. In order to gain more insight in these features, we have investigated a single AC powered dielectric barrier micro-discharge filament in contact with a water film, by means of ICCD imaging and optical emission spectroscopy. In contrast to dielectric barrier discharges with solid electrodes, a plasma spot is continuously observed at the water electrode during the entire voltage cycle [2]. Moreover, when the water serves as the momentary cathode, the discharge evolution displays a clear similarity with resistive barrier discharges, where a stable cathode fall region is formed in proximity of the liquid surface [2]. Since both observations are atypical for the case of solid electrodes, the underlying physical mechanisms are most likely unique to a liquid electrode. Surface deformation and droplet formation, for instance, can enhance the local electric field, which facilitates the formation of a cathode fall at the liquid surface. Next to that, evaporation and solvated ion desorption influence the plasma gas and can therefore alter both the local and general plasma properties. The similarity with resistive barrier discharges suggests the decisive role of the liquid resistivity. However, also a possibly distinct electron emission mechanism for liquids needs to be taken into consideration [3].

References

[1] P. Bruggeman, et al., *Plasma Sources Sci. Technol.* **25**(5), 053002 (2016).
[2] P. Vanraes, A. Nikiforov, A. Bogaerts and C. Leys, *Sci. Rep.* (under review).
[3] P. Bruggeman, and C. Leys, *J. Phys. D: Appl. Phys.* **42**(5), 053001 (2009).

1-3.O

DIFFUSION AND MICROSCOPIC CHARACTERISTICS OF LENGTH, TIME AND RATE OF TRANSFER OF SINGLY CHARGED IONS IN INFINITELY DILUTE SOLUTIONS IN MONOETHANOLAMINE

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Microscopic characteristics of length ($\bar{d}$)**,** time (τ) and transfer (hopping) rate (V) of 12 ions in monoethanolamine (MEA) at 298, 15 K were calculated. The calculation was made according to [1, 2] for aqueous [1] and alcoholic [2] solutions containing these ions. The data needed for the calculation are taken from [3].

Monoethanolamine, as well as water and primary alcohols, is a solvent with a spatial network of H-bonds. Therefore from the analysis of the results of calculation of values $\bar{d}$, τ, V the following regularities have been established similar for aqueous and alcoholic solutions with some differences:

1. Previously [1, 2], we found that parameter $\bar{d}$ reflects the real behavior of ion in solution and correlated with type of ion solvability by Samoilov [4]. For positive solvated ions $\bar{d}/r_i > 1$, $(\bar{d} - r_i) > 0$; for negative solvated ions – $\bar{d}/r_i < 1$, $(\bar{d} - r_i) < 0$ (r_i – ion structural radius). Therefore value $\bar{d}$ should not be considered as a radius of ion in solution. Based on this we proposed to replace the concept of "ionic Stokes radius" by the length of diffusion displacement of ion $\bar{d}$ [1, 2]. In MEA ions Rb^+, Cs^+, Me_4N^+, I^- are negatively solvated and ions Li^+, Na^+, K^+, Et_4N^+, Bu_4N^+, Cl^-, Br^-, BPh_4^- are positively solvated.

2. Hopping time (τ) is increasing and hopping rate (V) is decreasing in a series Cs^+, Rb^+, K^+, Me_4N^+, I^-, Na^+, Cl^-, Et_4N^+, Bu_4N^+, Li^+, BPh_4^- ions.

3. The isotherm $(\bar{d} - r_i) - 1/r_i$ for cations is described by a curve with a minimum similar the dependence $\Delta E_i - 1/r_i$ [3].

4. Value $\bar{d}$ in MEA for halide ions approximately 1 Å more than in water and with increasing of ion structural radius decreases, which is associated with the enhancement in a series H_2O-MEA and with weakening in the row Cl^-, Br^-, I^- of near solvation.

References

[1] V.I. Bulavin, I.M. V'yunyk, Ya.I. Lazareva, *Ukr. J. Phys*., **62**, 769 (2017).

[2] Abstracts of the 7th International Conference "Physics of liquid matter: modern problems", May 27-30, 2016, Kyiv, Ukraine. – P. 12.

[3] M.N. Rodnikova, T.A. Nosova, V.G. Markova, K.T. Dudnikova *Doklady Akademii nauk*, **327**, 96 (1992).

[4] O.Ya. Samoilov, Struktura vodnyh rastvorov jelektrolitov i gidratacija ionov, USSR Acad. of Sciences Publ., Moscow, 1957.

1-4.O

THE SIMILARITY AND DIFFERENCES IN THE BEHAVIOR OF THE THERMODYNAMIC PROPERTIES OF MONOHYDRIC ALCOHOLS, WATER AND ARGON ON THEIR COEXISTENCE CURVES

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There is an opinion that the properties of water and alcohols differ significantly from those for argon. It was formed under the influence of the fact that the properties of argon are determined by spherically symmetric potentials, in which the attractive part is due to dispersion forces, and the repulsion is only slightly different from that for hard spheres.
The work is devoted to the discussion of similarity and difference in the behavior of the simplest thermodynamic quantities for monoatomic alcohols and water – the fraction volume per molecule and evaporation heat. It is shown that the coexistence curves for all alcohols of methanol series and water have argon-like structure. The analogous conclusion is also made for the evaporation heat of all studied liquids. It is established that the small differences in the behavior of these characteristics for alcohols and water from those for argon are caused by the influence of H-bonds in them. The general method for the separation of the H-bond contributions to the fraction volume and evaporation heat is proposed. The optimal choice of the normalization temperature is considered in detail. It had been shown that values of the latter corresponds to $t_n \le 0.98$, i.e. these temperatures are outside of the critical fluctuations region. The determination of the averaged number of H-bonds per molecule is in details considered.
The approach we propose is model-free and relies only on the fact that small differences in the behavior of the coexistence curves can only be related to the most important characteristics of the H-bonds system.

Poster session

1-1.P

RAMAN SPECTRA AND AB INITIO CALCULATION OF A STRUCTURE OF AQUEOUS SOLUTIONS OF LIQUID WATER

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Analysis of the polarized Raman spectra allows one to make a conclusion that in the diffuse OH-band it is possible to extract contributions of symmetric and anti-symmetric vibrations of water molecules. $I_{\perp}(\nu)$ component with maximum at 3340 cm^{-1} is asymmetric in the low-frequency part ant it has a simplest shape of a wide band. $I_{||}(\nu)$ component possesses a degrade structure. While moving along the non-polarized band 3000-3800 sm^{-1} towards higher frequencies the depolarization ratio varies from rather small value to maximal one. The same conclusion can be made on the base of results of quantum-chemical calculations. We carried out quantum-chemical calculations to determine the structure of water aggregates. Calculations were performed for 10 units of water molecules. From results of experimental simulation of gas – liquid phase transition we can conclude that in liquid alcohols the diffuse band in the region of wave-numbers of 3400 sm^{-1} is connected with clasters of 4-5 molecules, which are formed due to intermolecular H-bands. One can logically suppose that analogous clasters are formed also in liquid water. For such structures we performed quantum-chemical calculations of not only the binding energies of molecules in the clasters, but also by modeling the Raman spectra. Vibrational bands, formed by each system, are significantly broadened. This fact we connect with the dephasing of intra-molecular vibrations, the probability of which increases in the process of formation of molecular clasters.

1-2.P

APPLICATION OF HEAT-SENSITIVE FLUORESCENT DYES TO DETERMINE THE SPATIAL AND TEMPORAL TEMPERATURE DISTRIBUTION IN LIQUID MEDIA

N.Gaiduk, N.Red'kin, A.Yakunov

In many technological processes and in biomedical applications, it is important to know the spatial and temporal distribution of temperature in a heated environment. Usually there is a need to control the local temperature by a non-contact method. Traditionally, the temperature is controlled by pyrometric measurements. However, for a wide range of technological processes and biomedical applications, the pyrometric method is not sensitive enough.

It is well known that the fluorescence spectra of some organic dyes solutions are very sensitive to temperature. In the present work, the aqueous and glycerol solutions of the organic dye of rhodamine 6G were used as a non-contact temperature sensor. Two parameters of the fluorescence spectrum showed a single-valued temperature dependence over a wide range of temperatures: the wavelength at the maximum of the spectrum and the asymmetry of the spectral band. At not very high temperatures these dependences are almost linear. This behavior completely corresponds to the existing concepts, since the temperature dependence of fluorescence spectra of solutions is essentially due to the relaxation kinetics of the solvent.

The fluorescence spectrum of the sample was excited with a semiconductor laser (405 nm, 50 mW) and detected by a low-dispersion UM-2 spectrometer. In output plane of spectrometer the CCD camera has been planted and connected with computer. Capture video and preprocessing of spectrum was carried out with help of open source software ImageJ.

The dye solution in glycerin was heated to 300 ° C in a microwave oven. Temporal changes in the parameters of the fluorescence spectrum corresponded to the calculated heating dynamics and showed good correlation with the operating mode of the microwave oven.

An aqueous solution was used to control the spatial and temporal temperature distribution in a flat (d = 10 mm) cuvette upon contact with a surface heated to 70 ° C. The dynamics and the spatial profile of the temperature distribution corresponded to the calculated data.

1-3.P

CALCIUM AND MAGNESIUM STEARATES VS. STEARIC ACID: DETAILS OF COMPLEXES FORMATION AND MEMBRANOTROPIC ACTION

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Calcium stearate (CaSt) and magnesium stearate (MgSt), as well as stearic acid (StA), are widely used excipients in a number of modern drugs. Complexes formation between drug constituents can affect drug therapeutic action at multiple levels, including membrane penetration. As it was shown in our previous calorimetric studies, individual membranotropic action of the substances is ranged as CaSt < MgSt < StA. Being added to dipalmitoylphosphatidylcholine (DPPC) model membrane together with antibacteial substance cycloserine (CyS), both CaSt and MgSt, as distinct from StA, induced non-linear effects in the membrane.

In order to elucidate these findings, further studies seemed to be necessary. Taking into account the substances location in DPPC membrane, with their hydrophobic moieties incorporated into lipid core and hydrophilic parts exposed to lipid/water interface, one can note that their hydration properties could be very important. Indeed, it was established that membrantotropic action of the excipients examined are in invert correlation with their hydration ability determined by means of isothermal sorption technique. Then, FTIR spectroscopy was involved to shed light on the possibility of complexes formation between CyS and the stearates in DPPC membrane. Disappointedly, the characteristic MgO and CaO bands appeared to be weak and overlapped by much stronger νCH_3 and δCH_2 bands, so no valuable information was obtained.

The electrospray ionization (ESI) mass spectrometry (MS) study of intermolecular interactions of CyS with StA in the model system cycloserin+stearic acid (1:10 molar ratio) in methanol was also performed. Along with the ions characteristic of the individual components of the mixture $[CyS{\bullet}H]^+$ at m/z 103.2 and $[StA{\bullet}Na]^+$ at 307.5, a weak peak of protonated molecular cluster of cycloserine with stearic acid $[CyS{\bullet}StA{\bullet}H]^+$ at m/z 387.7 was observed in the mass spectrum, which points to the possibility of noncovalent complexation of CyS with StA and their derivatives in the polar solvent.

1-4.P

TIME AND STOCHASTIC PARAMETERS OF THE DISRIUTION FUNCTION OF THE PROBABILITY DENSITY OF THE SPECTRA OF CAPILLARY WAVES OF NEAR SURFACE FLUID LAYERS

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The work is devoted to the study of stochastic properties of the free surface of an aqueous medium by measuring the power density spectra of thermal fluctuations existing on the free surface of a liquid (capillary waves). The aim of the research is to determine the temporal and stochastic characteristics of the probability density distribution function of the parameters of the capillary wave spectra of thin liquid layers to determine the characteristics of the effect of electromagnetic fields on the conformational characteristics of molecules dissolved in a liquid.

The object of the study was water distillate and aqueous solutions of nicotinamide adenine dinucleotidef (NADH), which is a derivative of vitamin B3 (niacin). The measurements were carried out using the optical heterodyning method. To probe the surface of the liquid, we used the radiation of an LG laser-72-II with l = 0.63 μm with a power of 3 mW. In the computer processing of the measurement results, the programs Origin0.5.2.49155 and Delphi XE8 were used. A Doppler shift of the frequency of light not elastically scattered by the free surface of the liquid was registered. The stochastic properties of the free surface of a liquid were determined by analyzing the energy spectrum of capillary waves of the free surface of a liquid. The results of the studies are illustrated in Fig.1.

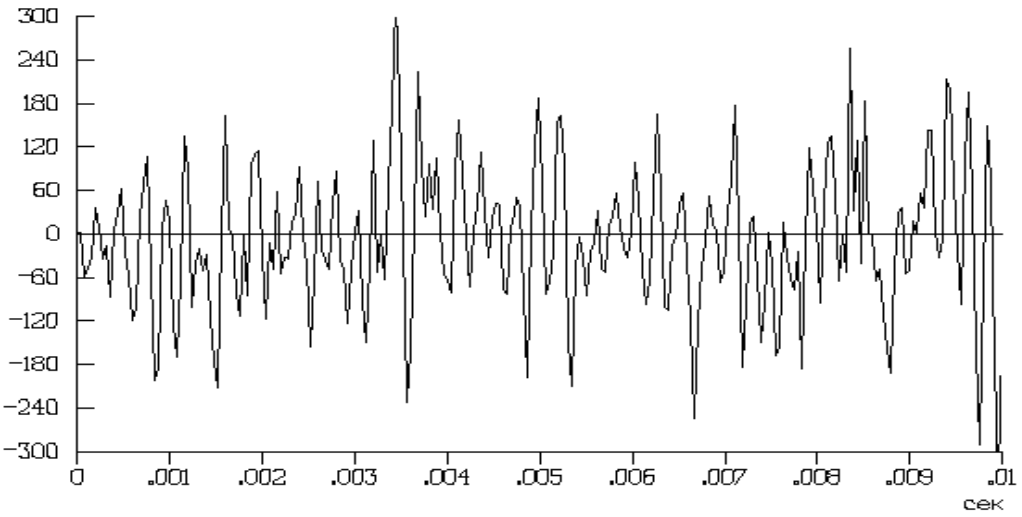

Fig.1. The time dependence of the signal reflected from the free surface of the distillate of water, which is proportional to the square of the amplitude of the capillary waves.

It was used that the magnitude of the amplitude of capillary waves is determined by the result of the competition of processes of their fluctuation jump excitation and macroscopic relaxation processes of a dissipative nature.

Conclusions. The parameters of the power density spectra of capillary waves of a liquid and their dependence on the concentration of dissolved NADH were established. For distilled water, it has been established that the power density spectrum of capillary waves existing on the water surface, measured during 1s, has an additive character. It consists of several successively existing in time elementary excitations with a duration of 1-5 ms, which have a high Q-factor. The function of probability distribution of the lifetime of such excitations was established and the minimum range of time for observing the water surface was determined, during which the form of this function does not change

1-5.P

DEFORMATION OF A LIQUID PARTICLE WHICH IS MOVING IN A NON-MIXED VISCOUS MEDIUM

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One of the methods of granular products manufacturing from melts or solutions of substances is a monodisperse fragmentation of capillary jet into droplets of the same size with their subsequent heat treatment to stabilize their form. An important problem of the monogranulation process organization is to ensuring the conditions under which the drops forms will be close to spherical. If the dynamic loads acting on the liquid particle from the side of the viscous medium in which it moves will exceed the forces of surface tension, the spherical droplet can not only deform, but also destruct. To determine the conditions under which a form of drop remains spherical, the problem of the motion of a liquid droplet in a viscous medium under the action of gravity is solved, taking into account the possible deformation of its surface. The problem is described by the system of Navier-Stokes equations for the droplet liquid and for the viscous medium in which it moves. On the surface of the drop, the velocities of the two media are considered equal, and also set the equalities of the tangential and normal stresses, taking into account the presence of surface tension forces. As a result of solving the problem and processing the results obtained, the dependences of the equilibrium velocity of the droplet and the degree of its deformation on the determining dimensionless criteria, to which the Reynolds and Weber numbers relate, are obtained. If the Weber number does not exceed 2, the form of the moving drop is near spherical. At Weber numbers exceeding 11 ... 12, the droplet surface loses stability and the drop is destroyed. In the range of Weber numbers from 2 to 11 ... 12, the drop acquires a shape close to ellipsoidal. Comparison of the results of the numerical solution of the problem with the results of the conducted experiments indicates that they are in satisfactory agreement.

THE VISCOELASTIC AND RELAXATION PROPERTIES OF AQUEOUS SOLUTIONS OF DECYLPYRIDINE CHLORIDE (DPCL)

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The study of the phenomena of self-assembly of supramolecular structures in liquid media, where various liquid-crystal states with the participation of organic molecules arise, indicate an important feature of these processes, that the main physical variable of the state is the concentration of the dissolved substance in the system. In the case of solutions of surfactants, such a system is a micellar state that occurs when a critical micelle concentration (CMC) is reached; micelles appear, and with a further increase in concentration, the system passes to different structural transitions.

One of the most effective methods for studying the mechanisms of micelle formation is acoustic spectroscopy, which makes it possible to record processes occurring in liquids with characteristic times of 10^{-6}-10^{-12} sec.

We investigated the viscoelastic and relaxation properties of aqueous solutions of decyl pyridine chloride (DPCL) by acoustic spectroscopy and rheology. Solutions with concentrations of 0.06 were studied; 0.1; 0.15; 0.2; 0.4; 0.8; 1.0; 1.67; and 2.0 mol/l. The amplitude coefficient of sound absorption was measured by a pulse method of varying distance in the frequency range from 3 to 2500 MHz with an error of 2 to 5%, the sound propagation velocity (s) was measured by the pulse-phase method with an error of 0.1%. Density was measured by a psychometric method with an error of 0.05%. The shear viscosity was measured with a capillary viscometer with an error of 1-2%. Measurements α, c, p and μs were performed along the liquid-vapor equilibrium curve in the temperature range 278-353 K.

The results of the measurements show that the density behavior in the investigated objects is linear, i.e. decreases monotonically with increasing temperature, increases with an increase in the surfactant concentration, ηs increases with an increase in the surfactant concentration, and also with a decrease in temperature.

The temperature dependence of the velocity of sound propagation shows that, like water, it increases with increasing temperature and passes through a maximum.

The curve for the concentration dependence of the sound propagation velocity in aqueous solutions of DPSI passes through a maximum in the concentration range 1.5-1.8 mol/l. This fact, in our opinion, can be explained as follows. As the concentration of DPSI increases, the number of micelles increases. At concentrations of $\varphi \leq 1.67$ mol/l, spherical micelles are combined into rodlike ones, similar to coins, and the viscosity of such a system increases sharply. At concentrations of>1.67, elongated rod-shaped micelles form a structured colloidal system in the entire volume of the solution, forming a mesomorphic phase.

The nature of the temperature dependence of the parameters Ai, bi, and η_{vi}/η_s for the investigated systems indicates that the observed acoustic relaxation can be caused by the processes of structural rearrangement, the low-frequency relaxation region is caused by the formation and decay of aggregates consisting of micelles, and the high-frequency relaxation by structural rearrangements .

1-7.P

THE RELAXATION PROPERTIES OF TRITON TX-100 AND AQUEOUS SOLUTIONS OF TRITON TX-100

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Despite numerous experimental work on micellar solutions and theoretical studies, the nature of the process of micelle formation is still a subject of debate. To obtain information on physical properties in such systems, the use of modern methods of physical and physicochemical analysis is required.

We investigated the relaxation properties of an individual nonionic surfactant (oxyethylated 1.1.3.3-tetrabutylphenol with a degree of oxyethylation of 9.5, the general formula C8H17C6H4 (OCH2CH2) 9.50H, known as Triton TX-100) and its aqueous solutions of concentrations (mol/liter): 16.9 • 10-5, 24 • 10-5, 89 • 10-5, 20.2 • 10-4, 24 • 10-4, 6.7 • 10-3 1.19 • 10-2.

The amplitude coefficient of sound absorption was measured by a pulse method of varying distance in the frequency range from 3 to 2500 MHz with an error of 2 to 5%, the sound propagation velocity (s) was measured by the pulse-phase method with an error of 0.1%. Density was measured by a pycnometric method with an error of 0.05%. The shear viscosity was measured with a capillary viscometer with an error of 1-2%. Measurements α, c, ρ и η_s were performed along the liquid-vapor equilibrium curve in the temperature range 278-353 K.

Analysis of the results of measurements of ρ and ηS showed that at a constant temperature, with increasing concentration of NPAW, the values of the density and viscosity values increase, while at p = const they decrease with increasing temperature.

The speed of sound in individual NPCs decreases linearly with increasing temperature. The temperature dependence of the sound velocity in the investigated aqueous solutions of NPAW, as in water, is of an extreme nature. Such a character of the temperature dependence of the sound velocity can be due to a change in the density and adiabatic compressibility (βS) with a change in the structure of the solution.

On the concentration dependence of the speed of sound propagation in aqueous solutions of TX-100 at T = const, three regions appear.

The first region up to a concentration of 0.7 KCM is characterized by a slight decrease in the speed of sound. The second area is observed with a further increase in the concentration of TX-100 to a value of 1 CMC. In this case, there is a sharp decrease in the speed of sound. The third region from 2 KKM to ~ 10 KKM is characterized by a close κ linear monotonic decrease in the speed of sound. In this region there are micelles that do not interact with each other. With a further increase in the concentration of TX-100, the sound velocity begins to increase monotonically.

The displacement of the temperature of the maximum of the sound velocity in the investigated aqueous solutions with an increase in the concentration of surfactants is apparently due to the fact that the water molecule is forced to orientate on the surface of the micelles. In this case, various micelle forms begin to form, the dimensions of which strongly depend on the concentration and temperature.

THE RELAXATION PROPERTIES OF AQUEOUS SOLUTIONS OF ABDM

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In connection with high technical and economic efficiency, surfactants are widely used in various industries, in particular, for the directed regulation of interfacial interactions in various disperse systems, for enhanced oil recovery, etc. Using the method of acoustic spectroscopy, one can obtain information on dynamic parameters flowing fast and ultrafast processes (characteristic times 10-4-10-10 s) in micellar solutions.

We investigated the relaxation properties of aqueous solutions of alkylbenzyldimethylammonium chloride (ABDM) by acoustic spectroscopy and rheology. Solutions with concentrations of 0.02, 0.05, 0.08, 0.1, 0.98 and 1.64 mol/l were studied. The amplitude coefficient of sound absorption was measured by a pulse method of varying distance in the frequency range from 3 to 2500 MHz with an error of 2 to 5%, the sound propagation velocity (s) was measured by the pulse-phase method with an error of 0.1%. Density was measured by a pycnometric method with an error of 0.05%. The shear viscosity was measured with a capillary viscometer with an error of 1-2%. Measurements p, c, α and μs were performed along the liquid-vapor equilibrium curve in the temperature range 278-353 K.

Analysis of the experimental data shows that in solutions with concentrations of 0.02 - 0.1 mol/l at constant temperature, α is proportional to the square of the frequency (f_2) in the entire frequency range and the temperature range investigated. On the basis of the experimentally obtained data, the sound absorption ($\alpha_{кл} \cdot f^{-2}$), due to the shear viscosity

$$\alpha_{кл.} \cdot f^{-2} = 26.3\eta_s \rho^{-1} c^{-3}, \quad (1)$$

as well as the ratio of the coefficients of bulk and shear viscosity

$$\eta_v \cdot \eta_s^{-1} = 4/3(\alpha - \alpha_{кл})\alpha_{кл}^{-1}. \quad (2)$$

As can be seen from the table, the character of the temperature dependence of $\alpha \cdot f^{-2}$, c, s and $\eta_v \cdot \eta_s^{-1}$ is the same as for pure water. This means that in the aqueous solutions of ABDM, as in water, excess absorption (αf^{-2} - $\alpha_{кл} \cdot f^{-2}$) is associated with irreversible rearrangement of the structure (the spatial arrangement of molecules, associates, water-surfactant complexes changes).

The presence of excess absorption indicates the existence of one or more relaxation processes at higher frequencies. Using the relation.

$$\tau_{ps} = \frac{\alpha}{f^2} \frac{c_0}{2\pi^2}, \quad (3)$$

the time of this relaxation process was calculated.

In ABMM solutions with concentrations of 0.98 and 1.64 mol/l, an acoustic relaxation process is observed, and the dependence of $\alpha \cdot f^{-2}$ on the frequency is described by the equation for one relaxation time.

$$\alpha \cdot f^{-2} = \frac{A}{1 + (f / f_p)^2} + B, \quad (4)$$

where A and B are the low-frequency and high-frequency limits $\alpha \cdot f^{-2}$, espectively, and fp is the relaxation frequency. The results of calculation of A, B and fp are given in Table. 2. Using relations (1) and (2), we calculated $\alpha_{кл} \cdot f^{-2}$, $\eta_v \cdot \eta_s^{-1}$, and the value of the relaxation force b was determined by the equation.

$$b = \frac{Acf_p}{\pi} \quad (5)$$

From the data obtained, it can be seen that in a solution of 0.98 mol/l, the values of parameters A and b decrease with increasing temperature, and f_p increase. This character of the temperature dependence of these parameters indicates that acoustic relaxation is due to the restructuring of the solution structure.

1-9.P

COMPLEX FORMATION IN METANOL/CHLOROFORM SOLUTIONS: VIBRATION SPECTROSCOPY AND QCE STUDY

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Methanol-chloroform solutions with different mixing ratios were studied by means of vibrational (IR absorbance and Raman) spectroscopy. Obtained spectra were analyzed by different techniques such as excess spectroscopy, two dimensional correlation analysis and multivariate curve resolution using alternating least squares (MCR-ALS). Our results indicate that methanol and chloroform do not mix completely at molecular level. Methanol-chloroform solutions behavior deviates strongly from ideal solution due to complex formation. MCR-ALS analysis of vibrational spectra shows that the investigated solutions consist of four kinds of species: 'pure' methanol, 'pure' chloroform and two types of molecular complexes. Molecular complexes exist in whole concentration range. Obtained spectral profiles of 'pure' methanol and 'pure' chloroform are identical to spectra of bulk species which means that their structure in solution are similar to corresponding ones in bulk methanol and chloroform.
Possible structures associates and molecular complexes were calculated using DFT with PBEh-3c functional which uses def2-SV(P) basis set and additional empirical dispersion correction D3. Information about optimized structures was further used for quantum cluster equilibrium (QCE) calculations. Obtained concentration dependences of mixture components correlate with experimental ones obtained by MCR-ALS.

1-10.P

MECHANISM OF EPITAXIAL GROWTH OF CRYSTALS FROM WATER SOLUTIONS

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The mechanisms of epitaxial growth of crystals from aqueous solutions associated with the participation of hydrogen bonds in this process is considered. The surfaces of layers formed on a glass substrate (microscope slides cat.NO.7101, clear glass) as a result of epitaxial growth of crystals from a solution of two types were investigated. The first type of aqueous solution (an aqueous solution of glucose with a concentration of 40%, PrJSC "Pharmaceutical Firm "Darnitsa", ATX B05CX1) is characterized by the formation of hydrogen bonds of the dissolved substance with water molecules. At forming crystals of the second type of aqueous solution (an aqueous NaCl solution with a concentration of 0,9% , SPrC "Yuria-Pharm", AA5027/1-1), such bonds do not form. The images of crystal layers from aqueous solutions of first and second types were obtained using the Integra Prima Basic atomic force microscope.
In the first case, clusters arise in solution, containing both particles of the dissolved substance and molecules [1]. These clusters diffuse to the substrate and settle on it, forming an epitaxial layer, which consists of ledges. These ledges are areas with a predominantly horizontal surface, separated by hollows with practically vertical walls and a depth on the order of the thickness of the layer. In the second case, the epitaxial layer is formed as a result of the settling of solute particles on the substrate. During this process the smoothing of ledges is occurred. So the slope angle of the epitaxial layer surface smoothly changes.

References

[1] L.A. Bulavin, Yu.F. Zabashta, E.O. Teliman, L.Yu .Vergun, *Colloid Journal*, **77(3)**, 1-6 (2015).

3D PES ASSOSIATED WITH DONOR HYDROXYL GROUP MOTIONS IN ACETILACETONE MOLECULE. STRETCHING AND BENDING OH VIBRATIONS STUDIED AT B3LYP/cc-pVTZ LEVEL OF THEORY

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Acetilacetone molecule (AA) – an important representative of compounds with intramolecular hydrogen bond. It shows a tautomeric equilibrium between the keto and the chelate enol forms. The last one is stabilized by a strong intramolecular hydrogen bond and is predominant in the gas phase [1]. Moreover it can exist in several geometric configurations (see Fig.1).

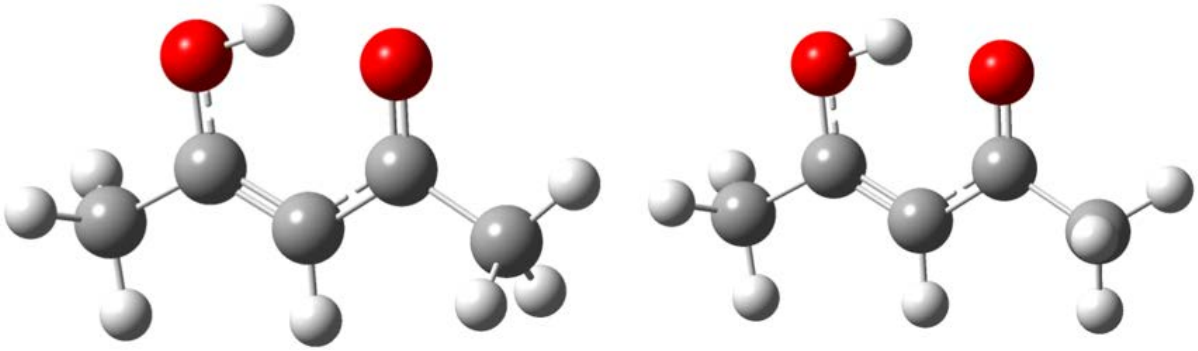

Figure 1. Equilibrium configurations of the acetilacetone molecule.

Thus studying of this molecule has theoretical and practical aspects. Taking in account the anharmonicity of the O-H group vibrations in AA one has to know multidimensional potential energy surface (PES) for large amplitude motion of the donor hydrogen atom. First of all, the equilibrium geometries of the AA were found at B3LYP/cc-pVTZ level of theory. Then the origin of the Cartesian coordinate system was placed at the donor hydrogen atom, X axis was directed along O-H bond, Y axis was located in the plane formed atoms of the hydrogen bridge, and Z axis supplements axes X and Y to the right-hand triple. Then the donor H atom was moved along X, Y and Z axis with 0.1 Å step while coordinates of all another atoms were fixed. 3D PES was calculated in all nodes of the 3D net in a parallelepiped with the sides $-0.4 \le X \le 0.6$, $-0.7 \le Y \le 0.7$, $0 \le Z \le 0.7$. To find frequencies of the donor hydroxyl group vibrations the following Schrödinger equation was solved using DVR method [2-6]:

$$-\frac{\hbar^2}{2\mu_{OH}}\frac{\partial^2\Psi}{\partial x^2}-\frac{\hbar^2}{2\mu_{OH}}\frac{\partial^2\Psi}{\partial y^2}-\frac{\hbar^2}{2\mu_{OH}}\frac{\partial^2\Psi}{\partial z^2}+U(x,y,z)\Psi=E\Psi$$

where $\mu_{OH}=\frac{M_O M_H}{M_O+M_H}$ – reduce mass of the H and O atoms, $x=\frac{X}{l_0};\ y=\frac{Y}{l_0};\ z=\frac{Z}{l_0};\ l_0=1\text{Å};$

As result of this calculations the frequencies of the all fundamental as well as overtones and combination vibrations of the donor hydroxyl group were found in 0-4200 cm^{-1} energy range. The calculated fundamental frequencies of the out of plane and in plane bending vibrations are equal to 958 and 1375 cm^{-1} respectively while the frequency of the stretching vibration is equals to 3109 cm^{-1} that in good agreement with experimental value (3090 cm^{-1})

References

[1] T. Chiavassa, P. Verlaque, L. Pizzala, P. Roubin, *Spectrochimica Acta*, **50A**, 343 (1994).
[2] D.O. Harris, G.G. Engerholm, W.D. Gwinn, *J. Chem. Phys*. **43** 1515 (1965).
[3] A.S. Dickinson, P.R. Certain, *J. Chem. Phys*. **49** 4209 (1968).
[4] R. Meyer, *J. Chem. Phys.* **52** 2053 (1970)
[5] J.C. Light, I.P. Hamilton, J.V. Lill, *J. Chem. Phys*. **82** 1400 (1985).
[6] D.T. Colbert, W.H. Miller, *J. Chem. Phys.* **96** 1982 (1992).

QUALITATIVE ANALYSIS OF CLUSTERIZATION IN WATER SOLUTIONS OF ALCOHOLS

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The work is devoted to the discussion of difference in the behavior of the simplest thermodynamic quantities for aqueous solutions of alcohols – the density and fraction volume per molecule. In such systems, there is a peculiar point [1,2].

The work discusses the features of clusterization in aqueous solutions of monohydric alcohols, i.e. belonging to the methanol series. The main focus is on the details of clustering in water-ethanol solutions. It is assumed that the degree of clustering depends not only on the nature of the interaction between molecules of ethanol and water [3], but also on the degree of ordering of the network of hydrogen bonds in water, which varies with the temperature and concentration of ethanol molecules. It is assumed that the volume occupied by an elementary cluster is less than the sum of the molecular volumes of the components forming this cluster.

In this paper discusses the peculiarities of clusterization in aqueous solutions of monohydric alcohols at higher and low concentrations than at a peculiar point. It occurs as a result of the formation of hydrogen bonds between water and alcohol molecules, whose energy is somewhat higher than the energy of hydrogen bonds between water-water and alcohol-alcohol molecules of the same type. It is assumed that in solutions form elementary clusters, the composition of which is fixed at concentrations smaller than at a peculiar point, and varies according to a certain law to the right of it. The extent of clusterization of a solution as a function of its concentration and temperature is determined.

Reference

[1] V. Ya. Gotsul'skii, N. P. Malomuzh, and V. E. Chechko. *Russian Journal of Physical Chemistry A*, **87**, 1638 (2013).
[2] L.A.Bulavin, V.Ya.Gotsulskiy, N.P.Malomuzh, V.E.Chechko. *Russian Chemical Bulletin,* **65(4)**, 851-876, (2016).

1-13.P

USING OF PLASMO-CHEMICAL TECHNOLOGIES FOR LIQUID RADIOACTIVE WASTE TREATMENT

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Under the regular exploitation of the nuclear fuel cycle objects, considerable quantities of liquid radioactive waste (LRW) with different composition and radionuclides activity are being generated: gamma- and beta-emitters: ^{95}Zr, ^{95}Nb, ^{60}Co, ^{59}Fe, ^{54}Mn, ^{51}Cr and ^{137}Cs, as well as the most alpha-emitters: plutonium, americium, curium, uranium and other nuclides, which require a special complicated technology of recycling, compaction and utilization for long-term storage. In case of accidents at a nuclear power station (Chernobyl NPS, Fukushima), a huge amount of radioactive elements, potentially dangerous for people and environment are being uncontrollably thrown away into environment. Presence of considerable amount of different organic and mineral components in radioactive water make the currently existing technologies of LRW treatment (method of evaporating, filtration, etc.) ineffective.

In this work there presented researches directed to the implementation of non-thermal plasma for effective treatment of different LRW with considerable concentration of organic components (SAS, SSAS, polymeric compounds, sylaxinacrilate binder). An original laboratory facility, which creates non-equilibrium non-thermal plasma in liquid which is saturated with a considerable amount of air and air with ozone, has been constructed. The main mechanisms and regularities of the considerable decrease of the content of hardly removable polymeric and other organic substances in radioactively polluted waters were studied in their dependence of the air and ozone concentration. It is shown that the main mechanisms of the organic substances oxidation are ozone, radicals, hydroxiles, ultraviolet radiation, which emerge in the process of non-equilibrium plasma appearance, and the emerging electrohydroshock and cavitation attack lead to the direct destruction of organics. The influence of the frequency, power, duration of an electrical discharge, leading to underwater plasma creation, on the effectiveness of the water treatment from radionuclides is studied.

The findings indicate that the use of the non-equilibrium plasma together with nanosorbates is perspective for discharge of different kinds of radionuclides from liquid radioactives wastes with the presence obstructive organic admixtures and can be a basis for creation of the industrial technology and equipment for effective and economically sound technology of the treatment of LRW at different industrial facilities.

1-14.P

STRUCTURAL-RHEOLOGICAL CHARACTERISTICS OF CONCENTRATED AQUEOUS AND ALCOHOLIC SOLUTIONS OF ELECTROLYTES IN THE TEMPERATURE RANGE (0-100)°C

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The authors have determined the structure of the near environment of cations and anions in solutions based on X-ray diffraction, neutron diffraction and rheological studies of aqueous and alcoholic concentrated solutions of 1-1, 2-1 and 3-1 electrolytes.

It was found that at concentrations of 1, 2, 3 or more moles per liter, the geometry of the near-surrounding of cations is close to the geometry of their environment in water-rich crystalline hydrates. The ordered arrangement of the solvent particles around the cations of transition metals (Ni, Co, Cu, Cr, La, Nd, Sm, Gd, Er) is characterized by a high binding energy due to the short-range donor-acceptor exchange interaction. The interaction of cations with molecules of solvent extends over distances which are several times larger than the size of the first solvation shell of the cation. At that, anions are mainly located on the surface of the first solvate's layer of the cation, which consists of molecules of solvent, and are the connecting links between adjacent spatially solvated cations.

Based on the analysis of rheological data and data on measurement of ultrasonic velocity, the average solvate numbers and the activation energy of the viscous flow of studied aqueous and alcohol solutions of electrolytes were determined. It was shown that the dependence of the logarithm of viscosity on the temperature of the studied systems can be approximated by several linear sections corresponding to definite values of the activation energy, which are characteristic for the given type of steady-state dynamically averaged structure of solution in a given temperature interval.

The calculated temperature dependences of the degree of temperature destruction of the liquid structure which were introduced by us correlate with the course of the change in the activation energy of their viscous laminar flow during heating.

1-15.P

TAUTOMERIC EQUILIBRIUM AND SLOW SELF-ASSEMBLING IN AQUEOUS SOLUTIONS OF LYOTROPIC CHROMONIC LIQUID CRYSTAL SUNSET YELLOW

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Temperature and composition effects on tautomeric equilibrium and slow self-assembling in various phases of Sunset Yellow FCF (SSY) aqueous solutions were studied by ^{1}H, ^{15}N NMR and Raman spectroscopy. The solutions were prepared according to the phase diagram in order to pass through all phase transitions between isotropic phase (I) and principal chromonic phases - nematic (N) and columnar (M) ones. It was shown that the tautomeric equilibrium in SSY is strongly shifted towards the hydrazone form. The corresponding equilibrium constant $pK_T = -2.5$ was calculated using the DFT SMD model. The dominance of hydrazone form was confirmed experimentally using the long-range ^{1}H–^{15}N correlation, widely known as HMBC. The observed chemical shift $\delta(^{15}\mathrm{N}) = -178$ ppm nicely correlates with the DFT results. The peak at 14.2 - 14.7 ppm found in ^{1}H NMR spectra in all phases can be attributed to the proton in the N–H…O bridge. It evidences that: i) the growing of SSY aggregates is accompanied by the segregation of water in the intercolumnar areas with no exchange with the N–H protons in the internal layers of the columnar stacks; ii) the life time of those aggregates is $\geq 10^{-7} - 10^{-8}$ s or even longer. The water confined in intercolumnar areas can be considered as the neat. Its molecular motion is changing at heating and crossing the border from M to N phases in similar manner as at the melting. The equilibration time for N+M $\rightarrow$ M is very long, most probably because of supramolecular restructuring, i.e. the growing of stack aggregates in M phase. If the sample is cooled down relatively fast to the temperature below N $\rightarrow$ M transition, the structural changes are behind, and the system falls to the supercooled state. Then the system evolves via slow self-assembling from this state to the equilibrium. This process can last over hours or even tens of days.

1-16.P

ζ-POTENTIAL IN THE STUDY OF AQUEOUS SOLUTIONS OF ALCOHOLS

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The anomalies of light scattering in some aqueous solutions allowed us to introduce a peculiar point. It was shown earlier that the peculiar point of dilute aqueous solutions of alcohols at concentrations of $x \sim 0.1$ molar fraction determines the fine structure in the refractive index values [1], the characteristic correlation times of scattered light in molecular scattering [2], and in scattering by suspended particles in solution [3].Neutral latex particles of ~ 10-50 nanometers in size with very small amounts in solution make it possible to define the properties of solutions on macro- and micro-scales.

It was also shown that in the vicinity of a peculiar point, an anomalously high time of establishment of the equilibrium state is observed. The equilibrium state is unstable [3] and leads to the formation of a micro-inhomogeneous (essentially dispersed) solution structure.

An important characteristic of liquid disperse systems is the electrical potential of the double electric layer (the ζ-potential) of particles suspended in solution. It is assumed that in water-alcohol solutions in the vicinity of the singular point the ζ potential can also exhibit specific behavior.

It is proposed to determine the concentration dependence of the ζ-potential in water-alcohol solutions near the peculiar point by two methods: the Method of Dynamic Light Scattering by changing the correlation time of autocorrelation intensity functions and the Laser Doppler Anemometer Method

References

[1] L.A. Bulavin, V.Ya. Gotsulskiy, N.P. Malomuzh, M.V. Stiranets, *Ukr. J. Phys.*, **60**, 1108-1114 (2015)

[2] V.Ya. Gotsulskiy, V.E. Chechko, Y.A. Melnik. *Ukr. J. Phys.*, **60**, 780-791 (2015)

[3] L.A.Bulavin, V.Ya.Gotsulskiy, N.P.Malomuzh, V.E.Chechko. *Russian Chemical Bulletin* **65**(4), 851-876, (2016).

RELATIONSHIP BETWEEN THE DEGREE OF HYDRATION OF THE SOLUTE AND THE EVAPORATION HEAT OF WATER

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The relationship between the degree of hydration and the specific heat of evaporation was shown by studies of the hydration of sucrose and the evaporation heat of water from its solutions. The DSK method was used to study the hydration of sucrose in the concentration range from 5.5 to 67.5 wt. %. It was found that the amount of hydrated water in the solution increases with increasing concentration. At the same time, the dependence of the hydration number on the solution concentration shows that the degree of hydration decreases with increasing sucrose content though the presence of free water in the solution [1]. One of the factors affecting the hydration of sucrose is the relative spatial orientation of its 8 hydroxyl groups. The preferred hydration interaction via hydrogen bonds with 6 equatorial hydroxyl groups is confirmed by the value of the first coordination number of sucrose hydration of 6.29 ± 0.18 mol/mol of sucrose, which was found for the state of the limiting water content of the solution.

Determination of the evaporation heat of water from solutions with an initial sucrose concentration of 12.5 wt. % was carried out at 40, 60 and 80 °C in a differential microcalorimeter of evaporation [2]. The basis of determining the specific heat of evaporation is the principle of synchronous continuous measurement of the mass of the sample and the amount of heat, which was consumed for evaporation during isothermal dehydration. Sucrose, chemically pure grade, and distilled water were used to prepare solutions. The measures were provided to prevent the possibility of development of microbiological activity in solutions. The mathematically expected relative error of determining the specific heat of evaporation of water is 0.49 % in the temperature range 30...90 °C, and the maximum possible error is 1.09%.

The experimental values of the specific heat of evaporation of water are represented by the curves of the dependence of the specific heat of evaporation ($R = r / r_{tab}$) on the solution concentration. The specific heat of evaporation r is close to the tabulated values r_{tab} only at the very beginning of the dehydration process ($R = \sim 1$), when the degree of hydration is ~ 20. As the solution concentration increases to ~ 65 wt. %, the evaporation heat is monotonically increasing, reaching an increment of 3-4%. In addition the degree of hydration of sucrose is reduced to ~ 6. Further concentration of solutions occurs as a result of the removal of hydrated water, directly associated with the equatorial hydroxyl groups of sucrose. The degree of hydration decreases, and the R dependence becomes steeper. The specific heat of evaporation of water in the concentration range close to saturation has values that exceed the specific heat of evaporation of clean water by 7-10%.

Comparing the dependence of the degree of hydration of sucrose and the specific heat of evaporation of water from its solutions on concentration, the physical model of dehydration can be represented as follows. Free water is removed to the concentration of the limiting water content of the solution by evaporation of water from sucrose solutions, containing both free and hydrated water. In this case, the change in the degree of hydration of sucrose continuously occurs in the solution in the direction of decrease, which leads to the transition of a part of the loosely bound hydrated water into free water. Energy is spent on changing the degree of hydration. This energy increases with increasing concentration of the solution. Thus, the internal latent heat of evaporation of water from the solution consists of the internal latent heat of evaporation of pure water and the energy expended to change the degree of hydration of sucrose. In connection with the increase in the binding energy between the molecules of water and sucrose with increasing concentration, the constituent of the hydration energy in the internal latent heat of evaporation of water from the solution also increases. Hydrated water evaporates from the solution after overcoming the limiting water content. This hydrated water is strongly bound to the equatorial hydroxyl groups of sucrose.

The fact of the dependence of the specific heat of water evaporation from solutions of sucrose on concentration raises the problem of its registration in the existing methods of thermal calculations of processes and equipment of the corresponding industries.

The reason of the increased energy expenditure becomes understandable during drying of sugar-containing materials of vegetable origin considering the concentration dependence of the degree of hydration of glucose and fructose, which is of the same type as sucrose.

References

[1] Mykhailyk V. Experimental study of sucrose hydration. Scientific works of Odessa National Academy of Food Technologies. Ministry of Education and Science of Ukraine. Odessa: 2006 (28). T. 2. S. 370-373.

[2] Dubovikova N., Snezhkin Yu.., Decusha L., Vorobyov L. Thermometric instrument of synchronous thermal analysis for determination of the specific heat of evaporation. Industrial Heat Engineering. 2013. T. 35, No. 2. P. 87-95.

1-18.P

USING OF PLASMO-CHEMICAL TECHNOLOGIES FOR ECOLOGICALLY SAFE TECHNOLOGY OF THE DISPOSAL OF RESISTANT ORGANIC CONTAMINATORS - POISONOUS CHEMICALS AND PECTICIDES

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Development of the chemical enterprises, intensification of crops growing with the purpose of their productivity increasing are connected with strengthening of man impact of chemical toxic agents and phytosanitary products on the biosphere and humans. Using of modern resistant organic contaminators (POC) - pesticides and poisonous chemicals - for plant pests extermination and crops defense lead to the environment pollution, and unclaimed poisonous chemicals and pesticides represent special hazard. The most dangerous ecotoxicants are resistant chloride-bearing preparations (DDT, TCAS, atrazine).

At the present time there are no effective methods and technologies of ecologically safe POC (pesticides, poisonous chemicals) disposal in the world practice. The widespread method of their disposal by burning is economically unprofitable and leads to a high risk of the secondary environmental pollution.

In this work there represented the researches directed to the using of non-thermal plasma for effective POC disposal with minimal risk for environment. With the help of constructed laboratory facility, consisting of a hydrodynamic cavitator unit, dielectric barrier plasma creation unit, non-equilibrium non-thermal plasma creation unit, a series of experimental works has been run under the different conditions of impact and different POC concentrations. There was revealed high effectiveness of POC disposal in liquids caused by the effect of synergism – mutual reinforcement of different impact mechanisms: cavitation destruction of organics, oxidation by ozone and hydroxiles, ultra-violet radiation, electro-hydropercussion impact. The main mechanisms and regularities of a considerable decrease of POC content were studied in their dependence on electric discharge power concentration, impulses duration and frequency, air and ozone concentration.

The findings indicate that synergic using of three different processes – plasma impacts together with hydrocavitation – is a perspective direction for creation of ecologically safe and economically effective technology of disposal of POC, pesticides and poisonous chemicals and can be a basis creation of the industrial technology and equipment.

ADIABATIC COMPRESSIBILITY OF AQUEOUS SOLUTIONS OF A POLYOLS NUMBERS

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One of the parameters is closely related to the structure of the liquid, is adiabatic compressibility. The experimental values necessary for the calculation of adiabatic compressibility are easily measurable according to the known equation $\beta_s = (\rho u^2)^{-1}$, and therefore the definition and subsequent analysis of behavior (βs), and derivatives from it, from temperature, condensation are a tried-and-true method of studying the structure of the fluid.

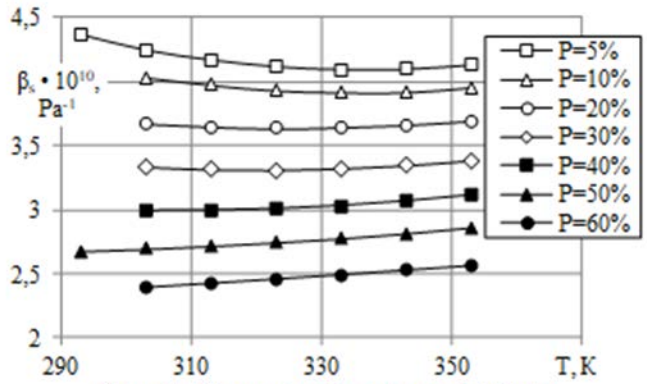

Figure 1 - Temperature dependence of adiabatic compressibility of aqueous solutions of xylitol

We carried out experimental studies of aqueous solutions of a number of polyols. Particularly of erythritol, xylitol, mannitol, sorbitol and dulcite in the range of temperatures of 283 - 353 K with concentrations from saturation to 1% by weight. Density measurements (ρ) were performed using a picometric method with an error of 0.05%. Methods of measuring the density and viscosity are described in detail [1]. The velocity of sound propagation was measured by a pulse - phase method at a frequency of 15 MHz, with an error of 0.5%, according to the technique [2].

Dependencies of adiabatic compressibility on temperature and concentration of investigation of solutions are similar to the temperature dependences of aqueous solutions of organic substances. In Figure 1, for example, the dependence is shown $\beta_s(T)$ for solutions of xylitol of different concentrations.

Depending β_s on the concentration of water, the behavior of organic substances is characteristic of aqueous solutions, namely, they have a "point" of the intersection. Characteristic is the fact that when the temperature rises, this "point" undergoes a shift towards lower concentrations of polyols. Such a drift becomes even more evident if we analyze the dependence of light adiabatic compressibility on concentration [3]. Figure 2 shows the dependence of molar adiabatic compressibility for solutions of xylitol at temperatures 293, 313, 333 K.

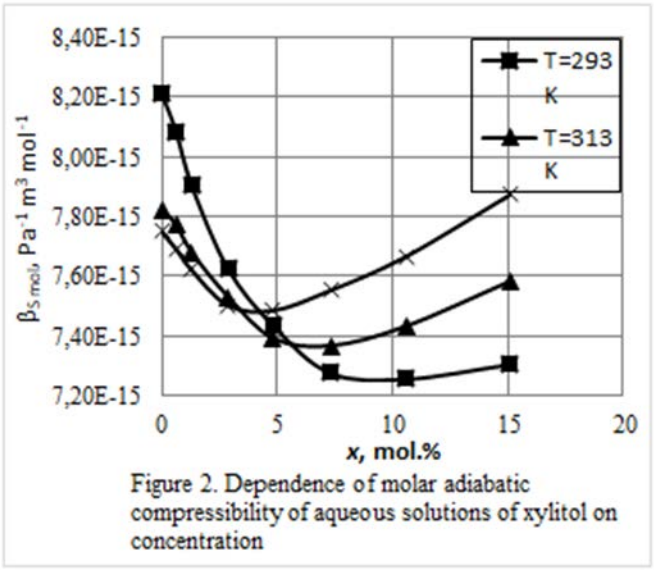

Figure 2. Dependence of molar adiabatic compressibility of aqueous solutions of xylitol on concentration

The indicated behavior of molar adiabatic compressibility from concentration will allow us to assert that in the aqueous solutions of polyols, the framework of co-operative hydrogen bonds of water undergoes a strong influence on the side of dissolved molecules.

The conducted studies allow to establish the limit concentration of polyol, which still allows the water framework to be preserved at a given temperature.

References

[1] Fundamentals of Rheology: Laboratory Workshop for students of the Faculty of Physics, specializing in "Molecular Physics" / Composition. L. A. Bulavin, I. I. Adamenko, G. N. Verbinskaya, D. A. Gavryushenko, Yu. F. Zabashta. - K.: Publishing and Printing Center "Kiev University", 2001. - 56 p.
[2] Rudenko, O.P. Experimental methods for determining the absorption of sound in liquids: a method. recommend [for students of physical specialties] / O. P. Rudenko, V. S. Sperkach. - Poltava, 1992. - 68 p.
[3] Grineva O.V. Structure of glycine-saturated water saturation close to the compressibility data / O.V. Grineva, E.V. Belyaeva // Journal of Structural Chemistry, **6 (52)**, 1176 – 1180 (2011).

DEVICE FOR DISINFECTION OF WATER BY USING ULTRAVIOLET RADIATION

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The method of ultraviolet disinfection of water is one of the physical, reagentless methods. The most effective impact energy of UV radiation from germicidal perspective occurs at a wavelength of 253.7 nm [1].
The purpose of the proposed technical solution is to simplify the design and reduce maintenance costs while maintaining the efficiency of disinfection of water.
In the known structures devices of productivity and the size of the Rays camera calculated by standard methods [2] using the experimentally determined volumetric dose H_V to inactivate various types of microorganisms. The disadvantage of this approach is that the volume dose H_V depends on the geometry of the camera for exposure and degree of mixing water during irradiation in laminar flow. To obtain the required dose of disinfection H_S , the size of the camera for radiation (diameter and length) should provide the required minimum radiation $E_{\min}$. Other areas will receive "excessive" exposure that only increases the reliability of disinfection.
The required dose H_S (W·cm^2) is achieved variation $E_{\min}$ (W·m^2) or time t (s):

$$H_S = E_{\min} \cdot t \tag{1}$$

Plant capacity for disinfection process is determined from the equation

$$V = \frac{E_2 \cdot l \cdot \pi \cdot R_1 \cdot e^{-k(R_1 - R_2)}}{H_S R_2} \left(R_2^2 - R_1^2\right) \tag{2}$$

Under these conditions, even in the case of laminar flow (when layers of water do not mix), layers of water that are far from the ultraviolet lamp, will receive the required dose for inactivation.

References

[1] A. Semenov and G. Kozhushko. Bactericidal irradiators for ultraviolet disinfection of indoor air, *European Applied Sciences*, **1(13)**, 226-228 (2013).
[2] A. Silva, N. Filho, M. Palha and S. Sarmento. Kinetics of water disinfection using UV-C radiation, *Fuel*, **110**, 114-123 (2013).

1-21.P

CONDUCTOMETRY OF WATER-ALCOHOL SOLUTIONS AND ALCOHOL NANOFLUIDS

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Peculiar points in water solutions of alcohols [1] and alcohol nanofluids (fluid-based suspensions of nano-sized particles) are widely researched and discussed. In particular, a new theoretical approach [2] was proposed recently which allows one to efficiently analyze the effective electrophysical parameters of a nanofluid based upon its microstructure, namely, the geometrical parameters and complex permittivity profiles.
The peculiarities of the concentration dependences obtained of nanofluids correlate with our experimental study of concentration dependences of the electrophysical characteristics (conductivity, electrical capacitance and dielectric permittivity) in equilibrium water-alcohol solutions. Special attention is paid to their behavior in the vicinity of the peculiar point defined as a point at which the intensity of molecular light scattering has a maximum. It is found that the electrophysical characteristics noticeably deviate from its reference value in the vicinity of the peculiar point $0.05 < x < 0.1$ (x - alcohol mole fraction). In the solution with the homogeneous distribution of water and alcohol molecules, there appear microregions with a slightly different type of the local structure. There emerges a region of special thermodynamic states.
Time of establishments of the equilibrium state after the imposition of an electric field at the conductometry of disperse systems wad investigated. When the field is applied, the equilibrium value of the parameters is achieved as a result of diffusion processes. Obvious, that the behavior of the electrophysical characteristics of water-alcohol solutions and alcohol nanofluids is of a general nature.

References

[1] V.Ya. Gotsulskiy, N.P. Malomuzh, V.E. Chechko, *JPC A*, **87**, 1638-1644 (2013)
[2] M.Ya. Sushko, V.Ya. Gotsulskiy, M.V. Stiranets, *Journal of Molecular Liquids*, **222**, 1051-1060 (2016)

1-22.P

VIBRATIONAL SPECTROSCOPY OF WATER: FROM CLUSTERS TO CONDENSED STATE

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Water is the most important substance for all living organisms on our planet, thus investigation of its structure is one of the most important problems, which has not been completely solved yet. The aim of research is to investigate the manifestations of the water structure in vibrational spectra at different temperatures in condensed state with special attention near a phase transition liquid-solid and to draw a conclusion about cluster structure of liquids at different temperatures using the results of matrix isolation experiments and quantum chemical calculations.
The confined hydrogen-bonded liquids are widespread in nature and important in both natural and engineered environments. The effects of nanoconfinement on the structure, dynamics and phase transitions in hydrogen-bonded liquids have a fundamental scientific importance and various implications in different areas. Thus, the influence of Argon matrix nanoconfinmets on vibrational spectra of water has been studied.
The presented IR absorption spectra were registered in the laboratory of Fourier transform infrared absorption spectroscopy at Physics Department of Vilnius University, Lithuania. These spectra were recorded using Bruker's VERTEX 70 FTIR spectrometer (condensed state) and IFS 113 Bruker's FTIR spectrometer (isolated in matrix) using LINKAM cryostat (model FTIR 600) thermo stabilizing equipment. Raman spectra of water were registered in the laboratory of Chebotarev Institute of Gerontology using the IsoPlane spectrograph and LINKAM cryostat (THMS600) thermo stabilizing equipment.

1-23.P

MODIFICATION OF WATER-SOLUBLE ANTITUMORAL PREPARATIONS WITH BY HELP RADIATION IRRADIATION OF SOLVENT.

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Actuality of researches is conditioned by the necessity of creation of non-destructive physical methods of modification of antitumoral preparations for the increase of their therapeutic efficiency

The of research objective - is the study and analysis of influence of previous irradiation of solvent on optical and therapeutic properties of solution of medicinal preparations of anthracycline and alkaloid rows for the increase of their efficiency.

The measurements used drugs doxorubicin ("Pharmacia Italia SpA" , Italy) and Conium (Weleda, Germany). The solvent used was a solution of sodium chloride in concentration 9 mg/ml, produced by LLC "Novofarm - Biosynthesis", Ukraine.

During optical studies, the spectral dependences of absorption (A) of solutions of dasgs in non-irradiated and previously irradiated by electrons of a solvent in the infrared light range were measured. The measurements were carried out on an IR-Fourier spectrometer Bruker IFS 66. The spectra were determined in the energy range (ε) [103 - 2 * 103] cm-1. The energy of the irradiating electrons was 1.0 MeV. The values of the dose of absorbed (I) irradiation were 5, 15, 25, 40, 80, 100 kGy. Correlation analysis of Pearson was used in the comparative analysis of absorption (A (ε, I)) of solutions of antitumor drugs. The interval ε is evenly divided by 200 points. The results illustrate the value of the correlation coefficients for the doxorubicin spectra: A (εε, 0 kGr), A (ei, 5 kGr)> = 0.37, A (εε, 0 kGy), A (ei, 15 kGr)> = 0 , 35; <A (εi, 0 кГр), A (εi, 40 кГр)> = 0,32; <A (εi, 0 kGy), A (εi, 80 kGr)> = 0.29, <A (εi, 0 kGr), A (εi, 100 kGr)> = 0.29. The critical value of the correlation coefficient at such a sample size and at the level of significance (accuracy of forecasting) 0.01 (1%) is equal to 0, 13. A similar result was obtained in the study of the conium. The study of the ability of high-energy electron irradiation of a physiological solution, as a solvent of a drug, to modify the pharmacological activity of the antitumor drug doxorubicin was investigated in vitro using the line of cancer cells of the lung carcinoma of Lewis (LLC). It was recorded that LLC incubation for 24 hours in the presence of doxorubicin, dissolved in a non-irradiated saline solution, resulted in a concentration-dependent decrease in the number of living cells. This behavior is due to inhibition of proliferation of tumor cells (cytostatic action) and / or their death (cytotoxic action) caused by the antitumor drug. At the same time, doxorubicin, dissolved in an irradiated saline solution, leads to an increase in cytotoxic / cytostatic effects, which is most pronounced at low concentrations: so, the number of LLC live cells at concentrations below 3 μM decreased by an average of 20% ($p < 0.05$) compared with the action of doxorubicin, dissolved in a non-irradiated physiological solution ..

Conclusions 1). Thus, preliminary radiation irradiation of the solvent, without substantially changing the medications (in all cases, the correlation coefficient exceeds the critical value), changes some of its properties in the oscillation range, which significantly depends on the conformational state of the molecules. 2)The ability of high-energy electron irradiation of a solvent to increase the pharmacological activity of antitumor drugs konium and doxorubicin (especially in the range of low concentrations of drugs) is established. The low variability of cell survival rates after incubation with doxorubicin in irradiated physiological saline as compared to the corresponding indices with non-irradiated solvent was registered.

1-24.P

MODELING OF POTENTIALS FOR INTERPARTICLE INTERACTIONS BETWEEN METHANOL MOLECULES

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Peculiarities of interparticle interactions between methanol molecules in the methanol vapor are investigated [1]. The bare potential is considered as a sum of repulsive, dispersive and electrostatic forces. It is supposed that H-bond has electrostatic nature (the irreducible contribution caused by overlapping of electronic shells is unessential) [2]. The dispersive interaction is approximated with London's formula, the electrostatic interaction is modeled by the multipole expansion up to dipole-octupole contribution. The multipole moments are assumed to be equal to their experimental values or quantum chemical calculations. The repulsion is modeled by power potential, parameters of which are fitted to the second virial coefficient and dimers parameters. Along with bare potential, the averaged potential of interparticle interaction is analyzed. It is shown that the repulsive potential has exponent n=28. The multipole potential, presented in this paper, is in details compared with the potential known as the OPLS [3]. Thermodynamic properties of methanol and water-methanol solutions are discussed.

References

[1] N. P. Malomuzh, M. V. Timofeev, *Condensed Matter Physics*, **20**, 43301:1-10 (2017).
[2] N. P. Malomuzh, I. V. Zhyganiuk, M. V. Timofeev, *Journal of Molecular Liquids*, **242**, 175-180 (2017).
[3] W. L. Jorgensen, *The Journal of Physical Chemistry*, **90**, 1276-1284 (1986).

1-25.P

STUDY OF INFLUENCE OF EXTERNAL FACTORS (HIGH TEMPERATURES, PRESSURES OR EXTERNAL RADIATION) ON PHYSICAL SYSTEMS

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A consequence of the influence of external factors (high temperatures, pressures or external radiation) on physical systems is the appearance in these systems of new components that differ from the components of the unperturbed system as the interaction energy, and the physical characteristics of the particles. Therefore, the formalism of the distribution functions is convenient from the point of view of the interpretation of both the structural changes that have occurred in the system and from the point of view of computing the change in the basic macroscopic characteristics of the system. Present work is dedicated to the investigation of temperature influence on those thermodynamic properties of liquid Ar, which are defined by the shift of chemical potential of the regarded system and its components under the influence of temperature. It was shown, that temperature of coexisting phases in stationary state leads to the shift of the parameters of phase transitions of the first order. Also the presented research studied the effect of temperature on the structural and dynamic properties of liquid Ar at high temperature and pressure by using the MD. A model relating the structural and dynamical properties of the Ar systems introduced. These data suggest that changes in temperature in a given interval leads to a change in the dynamic properties of liquid Ar. Analysis of the temperature and the time dependence of diffusion allowed to build a model representation describing the mechanisms of diffusion of the Ar systems and calculate their characteristic times. Qualitative analysis of the characteristic of the molecules of Ar, made from the the diffusion coefficient indicates the existence of various mechanisms of diffusion in Ar. To confirm the theoretical predictions, a qualitative comparison of the model with the existing experimental data on temperature influence on the physics properties of liquid Ar is performed.

1-26.P

PROPOSAL FOR THE USE OF THE PARALLEL ODRA RIVERBED (42ND TO 49TH KILOMETER OF THE RIVER) AS FLOOD PROTECTION

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Since the properties of water in riverbeds began to be influenced by anthropogenic factor, is the flood impact much stronger and less predictable. Research is focused on floods, which are caused by the injudicious alteration of the River Odra bed near the municipality of Albrechtičky in the Czech Republic. Changes in the riverbed caused overflow to the populated area instead of alluvial meadows. Suggested solution is the recovery of the parallel riverbed. As the flow regime has never been controlled in this area, it was necessary to carry out new measurement. In this case, it was methodology of flow measurement what has been used for the flow calculation. Flow measurement has been carried in five profiles. In some parts, where the channel has the smallest capacity, the measurement has been taken by the laser rangefinder. From these measured values was the maximal capacity determined by Chezy equation. Subsequently the hydrodynamic model HEC-RAS has simulated the proposal of flood control. According to the results of the Chezy equation and consumption curves has been found capacity of parallel channel about 3 – 7 m3.s-1 in the smallest parts. It means that it is able to take about thirty days of the Odra's flow. By using hydrological modelling were compared inundation areas during the current and newly proposed route and it has been found that the inundation area at the confluence of parallel troughs would decrease almost by the half. It would be appropriate to propose the connection of the River Odra bed and parallel riverbed in the flood area; it would cause decrease of the flow. The advantage of the proposal of flood control is certainly its near-natural character. It will improve reserves of surface water in the floodplain and ecological status of river.

References

[1] Krakovska, A, J. Novakova, J. Unucka, I. Melcakova, V. Lapcik, P. Andras A L. Klimsa. Proposal of Potential Flood Control. Carpathian Journal of Earth and Environmental Sciences [online], **12(1)**, 283 – 292, ISSN 1842 - 4090 (2017)

1-27.P

PROPOSAL OF POTENTIAL FLOOD CONTROL

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Since the properties of water in river beds began to be influenced by anthropogenic factor, is the flood impact much stronger and less predictable. Research is focused on floods, which are caused by the injudicious alteration of the River Odra bed near the municipality of Albrechtičky in the Czech Republic. Changes in the river bed caused overflow to the populated area instead of alluvial meadows. Suggested solution is the recovery of the parallel river bed. As the flow regime has never been controlled in this area, it was necessary to carry out new measurement. In this case it was methodology of flow measurement what has been used for the flow calculation. Flow measurement has been carried in five profiles. In some parts, where the channel has the smallest capacity, the measurment has been taken by the laser rangefinder. From these measured values was the maximal capacity determined by Chezy equation. Subsequently the proposal of flood control has been simulated by the hydrodynamic model HEC-RAS. According to the results of the Chezy equation and consumption curves has been found capacity of parallel channel about 3 – 7 $m^3.s^{-1}$ in the smallest parts. It means, that it is able to take about thirty days of the Odra's flow. By using hydrological modelling were compared inundation areas during the current and newly proposed route, and it has been found that the inundation area at the confluence of parallel troughs would decrease almost by the half. It would be appropriate to propose the connection of the River Odra bed and parallel river bed in the flood area, it would cause decrease of the flow. The advantage of the proposal of flood control is certainly its near-natural character. It will improve reserves of surface water in the floodplain and ecological status of river.

Section 2. Liquid Systems Contained in the Human Body

Oral session

2-1.O

THE EFFECT OF WATER ON THE FLEXIBILITY OF A SMALL PEPTIDE EXPLORED WITH MOLECULAR DYNAMICS SIMULATIONS

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We performed two short molecular dynamics simulations on glutathione (GSH) to understand the influence of molecules of water on the flexibility of the molecule. The results show that water certainly has a slight influence on glutathione as it "confines" its movement, however, this influence seems to be small and even negligible. All simulations were compared with experimental values.

2-2.O

JOINT ACTION OF DRUGS IN MODEL PHOSPHOLIPID MEMBRANES

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Model membranes based on hydrated phospholipids are examples of complex liquid systems with substantial medico-biological relevance. Therapeutic effects of drugs are largely dependent on "drug-membrane interactions", which involve interactions of drug molecules with both hydrophilic and hydrophobic moieties of phospholipids. When two or more different drugs are introduced, many specific effects emerge caused by direct or indirect interactions between drug molecules of different chemical nature. Alongside with spectroscopic methods, these effects can be studied by differential scanning calorimetry (DSC), with characteristics of thermotropic phase transitions showing strong sensitivity to these effects [1-4]. In this report, our previous experience is generalized, and several new cases in joint action of drugs are described, with manifestations of antagonism (decamethoxinum + aspirin [2, 3]), synergism (calcium and magnesium stearates + cycloserine) and competitive sorption (argentum + cuprum nitrates [4], dimethylsulfoxide (DMSO) + tilorone). Kinetic aspects of sequential introduction of the drugs are also considered. In particular, it was established that DMSO modulated kinetics of tilorone-membrane interactions, and the rate of tilorone diffusion was shown to be dependent upon the scheme of drugs administration.

References

[1] A.O. Sadchenko, O.V. Vashchenko, N.A. Kasian, etc., *Biophysics*, **62 (4)**, 570-579 (2017).
[2] O. Vashchenko, V. Pashynska, M. Kosevich and L. Lisetski, *Mol.Cryst.Liq.Cryst*, **547**, 155-163 (2011)
[3] N.A. Kasian, V.A. Pashynska, O.V. Vashchenko, A.O. Krasnikova, A. Gomory, M.V. Kosevich and L.N. Lisetski, *Mol.BioSyst*., **10**, 3155-3162 (2014),
[4] O.V. Vashchenko, A.O. Sadchenko, L.V. Budianska, L.N. Lisetski, *Biophysics*, **62 (2)**, 298-303 (2017).

2-3.O

EFFICIENT TWO-PHOTON LUMINESCENCE FOR BIOIMAGING USING POLYMER CONJUGATIONS OF GRAPHENE QUANTUM DOTS BASED MATERIALS

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In this study, examination results revealed that conjugated polymers containing nitrogen and sulfur atoms lead to a higher quantum confinement of emissive energy trapped on the surface of material (graphene quantum dot (GQD)-polymers), resulting in a high luminescence quantum yield and impressive two-photon properties. Additionally, the GQD-polymers generated nonreactive oxygen species-dependent oxidative stress on cells. Furthermore, we demonstrated the effective use of two-photon excitation-mediated high two-photon luminescence intensity in an acidic environment enableed GQD-polymers to act as a promising contrast probe. When cancer cells are labeled with specific antibody GQD-polymers conjugates, molecular-specific imaging can be performed deep into a tissue phantom with extremely high signal-to-noise ratios. In situations in which imaging depths are limited by the maximum available power that can be delivered to the three-dimensional (3D) bioimaging plane without causing damage to tissue, GQD-polymers might provide sufficient brightness to extend the maximum depth of imaging. Moreover, we demonstrated that the use of GQD-polymers can expand the capabilities of two-photon imaging to allow noninvasive 3D bioimaging of a variety of new molecular signatures.

Keywords graphene quantum dot-polymer; two-photon contrast agent; wo-photon excitation; two-photon luminescence; three-dimensional bioimaging

2-4.O

NONLINEAR KINETIC MODELS OF CELL-TO-CELL COMMUNICATION

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It is well known that cell-to-cell communication plays an important role in regulating of many physiological processes. As usual, it involves biochemical reactions, redistribution of fluids, changing electrochemical potentials and so on. Thus, it is natural that modeling of cell-to-cell communication is a complex and sophisticated task. The list of the most remarkable situations, which relate to cell-to-cell communication, includes (but is not limited to) such phenomena as calcium signaling [1] and synaptic transmission [2]. The last one is the crucial mechanism allowing neurons to spread signals. These are the cases when mathematical modeling can be applied. For example, passing a signal from one neuron to another involves several different stages. In general, it means that a signal should be passed through the synaptic cleft, which is the contact between two neurons. The neuron which sends the signal ends with the presynaptic membrane, and the neuron, which receives the signal, has a postsynaptic membrane. The synaptic cleft is the gap between the presynaptic and postsynaptic membranes. The signal activates the presynaptic membrane [3] and due to this mediator (which is a special substance) is released into the synaptic cleft. This mediator gets the postsynaptic membrane and interacts with membrane receptors. This in turn activates the postsynaptic membrane and leads to generating and spreading a new signal. So here we have a complex sequence of interactions. To model the total process we use a set of kinetic nonlinear models that allow us to find main functional characteristics of such systems as a synapse [4,5].

References

[1] M. Nivala, C.Y. Ko, M. Nivala, J.N. Weiss, Z. Qu, *Biophysical Journal*, **102**, 2433-2442 (2012).
[2] A.V. Chalyi A.V., A.N. Vasilev, E.V. Zaitseva, *Condensed Matter Physics*, **20**, 1, 13804: 1-12 (2017).
[3] S.O. Rizzoli, W.J. Betz, *Nature Reviews Neuroscience*, **6**, 1, 57-69, (2005).
[4] A.V. Chalyi, E.V. Zaitseva, *Journal of Physical Studies*, **11**, 3, 322-324 (2007).
[5] O.V. Chalyi, O.V. Zaitseva, *Ukrainian Journal of Physics*, **54**, 4, 366-370 (2009).

2-5.O

FREE AND CONFINED WATER AT THE ERYTHROCYTE MEMBRANES OF HEALTHY AND INVALID INDIVIDUALS: A MICROWAVE DIELECTROMETRY STUDY

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Blood is a concentrated suspension of red blood cells (RBC) and its physical properties are essential for proper circulation, oxygen delivery and nutrition of tissues. Especially its dielectric parameters are of relevance for medical diagnostics [1-3], cell separation, checking the deterioration of preserved blood, dielectric coagulometry and other medical applications. As it was shown by microwace dielectrometry (f=9.2 GHz), the real Re(ε) and imaginary Im(ε) parts of the complex dielectric permittivity ε of diluted suspensions of RBC and RBC ghosts of the blood sampled from patients with different types of cancer [2] and stroke [3] differ from those in healthy donors.

In this study Re(ε) and Im(ε) values have been measurement in the patients before and after X-ray and chemical treatment. The corresponding dependencies are presented in fig.1a,b. The differences between the healthy donors and patients are temperature dependent. After the successful treatment the dielectric properties return to the normal values. The proposed mechanism of the dielectric changes is based on the disease-specific modifications of the RBC membranes. The corresponding mathematical models are presented and discussed based on the experimental data.

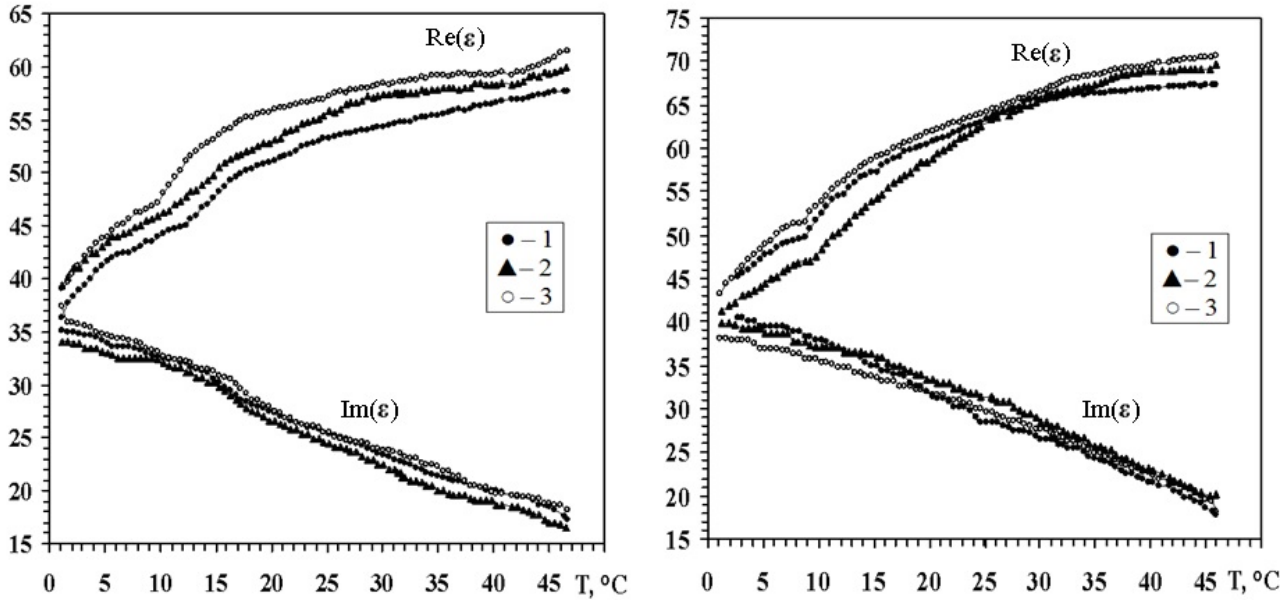

Fig.1. The dependencies Re(ε) and Im(ε) versus ambient temperature for RBC suspensions (a) and RBCe ghosts (b) measured on the control group (1) and groups of patients with breast (2) and lung cancer (3).

References

[1] Y. Hayashi, Y. Katsumoto, I. Oshige, et al., J. Non-Cryst. Solids **356**, 757–762 (2010).

[2] L. Batyuk and N. Kizilova, Book of Abstracts of the 14th Joint European Thermod. Conf., Budapest, 17-18 (2017).

[3] L. Batyuk, D. Astapovich, V. Berest and N. Kizilova, Book of Abstracts of Intern. Conf .”From molecules to functional materials”, Bialka Tatrzanska, Poland, 220-221 (2017).

OPTIMAL TEMPERATURE FOR HUMAN LIFE ACTIVITY

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The paper is devoted to the determination of the optimal temperature for the human life activity. It is assumed that the optimal temperature corresponds to extremal value of the oxygen flow from the lungs to human tissues on its vessels. It means that the ratio of saturation degree of the blood hemoglobin to the blood shear viscosity should be an object of our investigation. The blood shear viscosity is modeled by that for suspension, which the role of suspended particles belongs to red blood cells. It is shown, that such determined optimal temperature is equal to 36.6 0C that exactly coincides with the normal human temperature. The dependence of the optimal temperature human life activity on influence of alcohol and lactate is analyzed.

Notariously, the temperature's value of human life activity is 36.6 ^0C . It's distinctive temperature for existing water too. Under such temperature and normal pressure the water has lesser isobaric heat capacity. It makes more favorable conditions for thermoexchange in mammals, which tightly connect with oxidation process. The goal of present work is shown: "What kind of temperature is make an extremal value of oxygen transition from lungs to tissues?". It is assumed that the optimal temperature T_0 corresponds to extremal value of the oxygen flow from the lungs to human tissues $J_{O_2}(T,p,q)$ on its vessels:

$$T_0 \Leftrightarrow \max J_{O_2}(T,p,q), \quad (1)$$

which dependent from: 1) temperature: the degree of hemoglobin saturation $S_{o_2}\left(T,P_{osm},p,q\right)$ with determined density $n(T,p,q)$ in blood flow Q_B per unit time has changed from temperature and a partial pressure P_{osm} [1] (fig.1):

$$J_{O_2}(T,p,q)=Q_B(\Delta P)n(T,p,q)S_{O_2}(T,P_{osm},p,q) \quad (2)$$

and 2) from viscosity of blood, which determine as suspension's viscosity and expressed as:

$$\eta(T,p)=\eta_P(T,p)\Gamma(\Psi) \quad (3)$$

The formula brought with help cell method [2]. The optimal temperature of human vital activity determined by given of maximum:

$$\max F(T,P_{osm},p_0,q_0)\to T_0 . \quad (4)$$

Under normal conditions it determine by ratio

$$\max f(T,P_{osm},p_0,q_0)\to T_0 ,$$

while function $f(T,P_{osm},p_0,q_0)$ on different from $F(T,P_{osm},p_0,q_0)$ dependent only from shear plasma blood viscosity:

$$f(T,P_{osm},p_0,q_0)=\frac{S_{O_2}(T,P_{osm},p_0,q_0)}{\eta_p(T,p_0,q_0)} \quad (6)$$

Because the change of RBC volume we can negligible.

By using temperature dependence of shear plasma blood viscosity we got follow numeral value of function $f(T,P_{osm},p_0,q_0)$ (tab.1):

$T,\ ^0C$	23	30	37	44
S_{O_2}	0.98	0.95	0.92	0.88
η_p	2.2	1.8	1.5	1.45
$f(T,P_{osm},p_0,q_0)$	0.45	0.53	0.61	0.60

Really, the function $f(T, P_{osm}, p, q)$ assumes the maximal value under temperature $37\ ^0C$. By reason of reject an experimental dates of temperature dependence of η_p we can't determine an optimal temperature T_0 more exactly.

References:

B.Tremey and B.Vigue. Ann.Franc.Anesth.et Rean., 23, no 5, (2004) 474-481.
MicroVisc [http://www.rheosense.com/application/viscosity-of-blood-plasma-and-serum]

Poster session

2-1.P

USE THE NEUTRAL ANOLYTES FOR MONITORING FOOD QUALITY CONTROL

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Within the framework of EU the question of safety and quality of foods in a chain "from the field to the table" is regulated about by 160 directives. General principles are described in Regulation (EC) № 178/2002. Food products are all susceptible to microbial spoilage because of their chemical composition.

In our time, a new generation of biocidal solutions based on the electrochemical activated water is intensively developed. Particular attention is drawn to the so-called neutral anolytes, which have pH values close to neutral (pH 6.8 - 7.8) but have high oxidation-reducing potential (Redox = + 500 - 900 mV). Such anolytic contains active substances chlorinated acid (HClO), hypochlorite ion (ClO-), ozone, hydrogen peroxide, and other metastable compounds of the peroxide type containing active oxygen. Metastability is excellent quality of neutral anolyte(it does not leave contaminations, does not accumulate in the body and in the environment). Concentrations of active-reactive substances (0,02-0,09%) are significantly lower concentrations in the antiseptics of the old generation, which essentially reduces the probability of formation of toxic halogen-containing compounds.

Anolyte is an oxidizing agent due to a mixture of free radicals and has an antimicrobial effect among causative agents: Escherichia coli, Listeria monocytogenes, Salmonella, Staphylococcus, Yersinia enterocolitica, Clostridium perfringens, Campilobacter jejuni, that circulate among the population of agricultural animals. Particular interest was presented by the cultures of Salmonella: S.canada, S.paratyphi, S. eimsbuettel, S. california. On the basis of the got results facilities of warning of microbiological contamination of foods and realization of monitoring researches will be worked out.

We developed a compact, easy to use device for preparing aqueous neutral anolyte and analyzed the antimicrobial effect prepared by our neutral anolyte technology. On the basis of the obtained results, the means of prevention of microbiological contamination of food products and conducting of monitoring research will be developed.

2-2.P

USING OF PLASMO-CHEMICAL TECHNOLOGIES FOR LIQUID RADIOACTIVE WASTE TREATMENT

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Under the regular exploitation of the nuclear fuel cycle objects, considerable quantities of liquid radioactive waste (LRW) with different composition and radionuclides activity are being generated: gamma- and beta-emitters: ^{95}Zr, ^{95}Nb, ^{60}Co, ^{59}Fe, ^{54}Mn, ^{51}Cr and ^{137}Cs, as well as the most alpha-emitters: plutonium, americium, curium, uranium and other nuclides, which require a special complicated technology of recycling, compaction and utilization for long-term storage. In case of accidents at a nuclear power station (Chernobyl NPS, Fukushima), a huge amount of radioactive elements, potentially dangerous for people and environment are being uncontrollably thrown away into environment. Presence of considerable amount of different organic and mineral components in radioactive water make the currently existing technologies of LRW treatment (method of evaporating, filtration, etc.) ineffective.

In this work there presented researches directed to the implementation of non-thermal plasma for effective treatment of different LRW with considerable concentration of organic components (SAS, SSAS, polymeric compounds, sylaxinacrilate binder). An original laboratory facility, which creates non-equilibrium non-thermal plasma in liquid which is saturated with a considerable amount of air and air with ozone, has been constructed. The main mechanisms and regularities of the considerable decrease of the content of hardly removable polymeric and other organic substances in radioactively polluted waters were studied in their dependence of the air and ozone concentration. It is shown that the main mechanisms of the organic substances oxidation are ozone, radicals, hydroxiles, ultraviolet radiation, which emerge in the process of non-equilibrium plasma appearance, and the emerging electrohydroshock and cavitation attack lead to the direct destruction of organics. The influence of the frequency, power, duration of an electrical discharge, leading to underwater plasma creation, on the effectiveness of the water treatment from radionuclides is studied.

The findings indicate that the use of the non-equilibrium plasma together with nanosorbates is perspective for discharge of different kinds of radionuclides from liquid radioactives wastes with the presence obstructive organic admixtures and can be a basis for creation of the industrial technology and equipment for effective and economically sound technology of the treatment of LRW at different industrial facilities.

2-3.P

DYNAMIC SPECKLE ANALYSIS IN APPLICATION TO PHYSICS OF LIQUIDS AND CELL BIOPHYSICS

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Dynamic speckle as a flickering spotted field is observed when coherent light is scattered on a rough surface or in a turbid medium with time-varying parameters. Analysis of the dynamic speckle pattern may provide information about the processes taking place at the scattering medium. Numerous algorithms have been developed to analyze the evolution of dynamic speckles. Dynamic speckle metrology was successfully used in some biomedical, physical and chemical applications. We present two new applications using dynamic speckle analysis.

Previously [1] we showed how it is possible to investigate the pure liquids using dynamic speckles. Pure liquids are not able to form speckles on their own. But the spatial heterogeneity of the refractive index may affect the propagation of the light beam in the medium. If the input beam in the form of a static speckle field passes through a flat-parallel liquid layer, signs of dynamic behavior appear in the speckle pattern at the outlet. That is, a layer of transparent liquid performs modulation of the light flux.

As far as we know, we represent the first realization of the dynamic speckle method for studying the structural dynamics of pure H-bound liquids. In the first stage we show that a layer of pure liquid produces a modulation of the static speckle field. In the second stage, a correlation is established between the parameters of the dynamic speckle pattern and the characteristics of the H-bound liquids. Finally, we consider some approaches to the development of data processing algorithms using the original evolutional matrix formalism.

In another application, we used dynamic speckle analysis to study the biological dielectrophoresis - the movement of cells caused by an electromagnetic field in the millimeter range. The interaction of millimeter waves with living cells is a fundamental and still unsolved problem. Biological dielectrophoresis seems to be a subtle tool for investigating such interactions [2].

The coherent laser light is scattered on a thin optically non-uniform layer of cells in an aqueous medium. In the absence of external factors, the cells are in Brownian motion, which is manifested in the background dynamics of the speckle pattern. The inclusion of an external electromagnetic field changes the nature of the motion of the cells: the parameters of the dynamics of the speckle pattern change. Preliminary results show the effect of the frequency and power of radiation on the behavior of cells.

References

1. Pobiedina, V. and A. Yakunov. *Speckle decorrelation study of phase heterogeneous liquid medium*. in *SPIE Photonics Europe*. 2016. International Society for Optics and Photonics.

2. Pohl, H.A. and J.S. Crane, *Dielectrophoresis of cells.* Biophysical journal, **11**(9), 711-727 (1971).

2-4.P

MEMBRANOTROPIC EFFECTS OF LAURIC ACID, FENSPIRID AND KAOLINE IN MODEL LIPID MEMBRANES: IMPACT OF LIPID COMPOSITION

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Lipid composition is known to substantially affect membrane properties, which may relate to drug delivery and susceptibility. The aim of this study was to compare membranotropic effects of different dopants in model lipid membranes of various compositions.

Dopants with different membranotropic action were used: lauric acid (LA), a component of cell membranes with antimicrobial properties, anti-inflammatory drug fenspirid (F), and kaolin (K), a surface-active non-penetrative agent with both internal and external medical applications. Concentrations explored were up to 5 % w/w for F and LA, and up to 20 % w/w for K.

Three types of lipid membranes were used: (1) standard monolipid dipalmitoylphosphatidylcholine membrane (DPPC); (2) phospatidylcholine-phosphatidylethanolamine-cholesterol membrane (PC-PE-Chol) which mimics lipid composition of enterocytes; (3) ceramide-containing membrane (DPPC-Cer) which mimics lipid composition of skin cells membrane. Membrane phase transitions were studied by differential scanning calorimetry (DSC) in repeated cooling-heating scans. In order to characterize membranotropic action of a dopant, a set of thermodynamic parameters were obtained from DSC profiles, including the temperature of main phase transition, Tm, which appeared to be the most informative characteristic.

The greatest variety of changes was induced by LA, which was reflected not only in Tm, but also in enthalpy and half-width. The effect of Tm increase induced by LA was smaller in PC-PE-Chol membrane as compared with DPPC, and disappeared in DPPC-Cer membrane. On the contrary, strong Tm lowering effect of F remains almost unchanged, within the measurement accuracy, in all membranes. The most unexpected results were obtained for K. It caused non-monotonous concentration dependence of Tm, with minimum at ~ 7 %, in DPPC membrane, and an opposite run, with maximum at ~ 7 %, in PC-PE-Chol membrane. In DPPC-Cer membrane, saturation was observed.

The results obtained are interpreted in terms of molecular packing and hydration in lipid bilayers.

2-5.P

SYNERGETIC APPROACH TO INTERDISCIPLINARY DIALOGUE BETWEEN PHYSICS AND MEDICINE

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In this presentation, we will focus our attention to integration trends in education and science, which are associated with the strengthening of interdisciplinary connections, using the synergetics - an interdisciplinary science seeking to combine phenomena of different nature in open, nonequilibrium, nonlinear, complex systems - for a deeper understanding of the unity of laws in organic and inorganic world and society [1-4].

The main attention is paid to considering the following three examples of the application of synergetic models on the boundary between physics and medicine:

1st example: "Physics and medicine (oncology)". In this example, the synergetic similarity of nucleation processes and carcinogenesis will be considered (see detail in [5]).

2nd example: "Chemistry, physics, mathematics and medicine (cardiology)". In this example, spiral waves in the periodic reaction of Belousov-Jabotinsky and in the myocardium will be considered, as well as the cause of an instantaneous cardiac arrest established by N. Wiener and A. Rosenblute [6,7].

3rd example: "Physics and medicine (psychiatry, neurophysiology)". In this example, hexagonal structures will be considered in different systems, namely: in Benard cells, on the eye's retina in the case of Liao depression, in the system of grid-neurons being a mechanism of spatial orientation for people and animals (Nobel Prize in medicine or physiology in 2014) [2,8].

A list of monographs and papers on synergetics of natural sciences, being far from completeness, is presented below:

1.G. Nicolis, I. Prigogine. Self-organization in Nonequilibrium Systems - M .: Mir, 1979.
2. G. Haken, Synergetics - M .: Mir, 1980.
3. O.V. Chalyi, Synergetic Principles of Education and Science - K .: Vipol, 2000.
4. V.I. Sugakov, Fundamentals of Synergetics - K.: Oberig, 2001.
5. A.V.Chalyi, *Reports of Natl.Acad.Sci.Ukraine*, **9**, 170, (2012).
6. V.I. Krinskyy, A.S. Mikhailov, Autowaves – M.: Znanie, 1984.
7. AV Chalyi, Nonequilibrium Processes in Physics and Biology - K .: Naukova Dumka, 1997.
8. E.I. Moser, M-B. Moser, Seeing into the future. *Nature*, **469**, 303, (2011).

2-6.P

INTERACTION OF SOME STYRYL DYES WITH DNA AND ITS SPECTROSCOPIC MANIFESTATION

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Organic dyes are widely used in dye laser as active substance, in analytical chemistry for determination of micro quantity of various elements and in other area of the science and technology. In dependence from solved task are required those or other dyes. In particular, in medical and biological research for diagnosing various pathologies as fluorescent probes and labels used styryl dyes.

The purpose of present work is the investigation of the spectral-luminescent characteristics of the newly synthesized styryl dyes on the base of **Sbt** dye [1] in aqueous solutions without and in the presence of deoxyribonucleic acid (DNA) of the salmon.

It was found that with an increase in the concentration of DNA in the aqueous solution of **D-166**, **Dbt-5** and **D-179** dyes, the intensity of the absorption and fluorescence bands decreases to a concentration of 8×10^{-6}M. Beginning at a concentration of 1.6×10^{-5} M, a new band is observed in the absorption spectrum from the side of long waves.

At the same time, a bathochromic shift of 10-15 nm occurs in the fluorescence spectrum and the luminescence intensity increases by a factor of 3-6. For Sbt and S-6 dyes, the shape of the absorption and fluorescence spectra of aqueous dye solutions remains constant in the presence of DNA, and the fluorescence intensity is increased in two times.

Based on the experimental data for the aqueous solutions of the studied dyes without and in the presence of DNA, the main spectral-luminescence characteristics were calculated: extinction coefficient (ε), oscillator strength (fe), lifetime of the excited state (τ), quantum yield of fluorescence (B), frequency 0-0 transition ($\nu_{0\text{-}0}$), Stokes shift (SS) and biophysical parameters: binding constant (K) and concentration of binding sites (N). The nature of the observed phenomena is discussed.

References

[1] V.B. Kowalska, D.V. Kryvorotenko, A.O.Balanda, M.Yu.Losytskyy, V.P.Tokar, S. Yarmolyuk. *Dyes and Pigments* **67**, 47-54 (2005).

2-7.P

USING OF PLASMO-CHEMICAL TECHNOLOGIES FOR ECOLOGICALLY SAFE TECHNOLOGY OF THE DISPOSAL OF RESISTANT ORGANIC CONTAMINATORS - POISONOUS CHEMICALS AND PECTICIDES

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Development of the chemical enterprises, intensification of crops growing with the purpose of their productivity increasing are connected with strengthening of man impact of chemical toxic agents and phytosanitary products on the biosphere and humans. Using of modern resistant organic contaminators (POC) - pesticides and poisonous chemicals - for plant pests extermination and crops defense lead to the environment pollution, and unclaimed poisonous chemicals and pesticides represent special hazard. The most dangerous ecotoxicants are resistant chloride-bearing preparations (DDT, TCAS, atrazine).

At the present time there are no effective methods and technologies of ecologically safe POC (pesticides, poisonous chemicals) disposal in the world practice. The widespread method of their disposal by burning is economically unprofitable and leads to a high risk of the secondary environmental pollution.

In this work there represented the researches directed to the using of non-thermal plasma for effective POC disposal with minimal risk for environment. With the help of constructed laboratory facility, consisting of a hydrodynamic cavitator unit, dielectric barrier plasma creation unit, non-equilibrium non-thermal plasma creation unit, a series of experimental works has been run under the different conditions of impact and different POC concentrations. There was revealed high effectiveness of POC disposal in liquids caused by the effect of synergism – mutual reinforcement of different impact mechanisms: cavitation destruction of organics, oxidation by ozone and hydroxiles, ultra-violet radiation, electro-hydropercussion impact. The main mechanisms and regularities of a considerable decrease of POC content were studied in their dependence on electric discharge power concentration, impulses duration and frequency, air and ozone concentration.

The findings indicate that synergic using of three different processes – plasma impacts together with hydrocavitation – is a perspective direction for creation of ecologically safe and economically effective technology of disposal of POC, pesticides and poisonous chemicals and can be a basis creation of the industrial technology and equipment.

2-8.P

ASSESSMENT MECHANISM OF BLOOD FLOW IN VESSELS USING MAGNETIC RESONANCE TOMOGRAPHY

L.A.Bulavin, Yu.F.Zabashta, B.V.Batsak

The blood flow in the vessels is realized in the form of a pulse wave. The pulse wave, during spreading along the vessel, meets areas where the shape and size of the section change, as well as the sections containing branching. These areas play the role of obstacles on which the pulse wave is reflected.

It is generally accepted that the reflected waves that arise in this case are homogeneous. This statement is doubtful, since the presence of such waves would lead to a violation of the periodicity of the blood flow, which, however, is not actually observed.

Mathematical modeling of the blood flow was carried out, which showed that the reflected waves are inhomogeneous - damped at a distance from the obstacle, equal in order of magnitude to the diameter of the vessel. In this case, the periodicity of the blood flow is preserved.

It was found that in this case a linear relationship between the blood flow velocity and the cross-sectional area of the vessel should be observed.

The existence of such a relationship is confirmed by measurements performed by the MRI method for various vessels.

Based on the conclusion about the heterogeneity of the reflected waves, a formula is obtained that connects the arterial pressure in this section of the vessel with the rate of blood flow and the diameter of the vessel-the values measured by the MRI method. The pressure values in various vessels are calculated with a help of formula and data obtained from the MRI sequences.

2-9.P

CONFORMATION CHANGES OF HUMAN SERUM ALBUMINE UNDER TEMPERATURE EFFECT IN PHISIOLOGYCAL TEMPERATURE RANGE

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Water is essential for protein three-dimensional structure, conformational dynamics, and activity. Human serum albumin (HSA) is one of major blood plasma proteins, and its functioning is fundamentally determined by the dynamics of surrounding water. The goal of this study is to correlate the conformational dynamics of albumin to the thermal motions in water taking place in the physiological temperature range. We report the results of molecular dynamics simulations of temperature effect on the HSA macromolecule in aqueous solution. The dynamics of HSA macromolecule in aqueous solution has been simulated using the multifunction package HARLEM, which combines methods of molecular and Brownian dynamics. The crystallographic structure (PDB entry 1AO6) [1] of albumin at the resolution of 2.5 Å was used. The simulation of the temperature effect on the conformation stability has shown structural changes in secondary structures of HAS. Conformational changes take place in the components of the regular secondary structures, which are stabilized by hydrogen bonds. Most the structural rearrangements are observed in the α-helix.

References

[1] S. Sugio, A. Kashima, S. Mochizuki, M. Noda, K. Kobayashi, Crystal structure of human serum albumin at 2.5 Å resolution, *Protein Eng.* **12,** 439–446 (1999).

2-10.P

RAYLEIGH-TAYLOR'S DISSIPATIVE INSTABILITY AND ITS CONTRIBUTION TO THE FORMATION OF THE CONNECTION BOUNDARY AT THE ELECTRIC WELDING OF BIOMATERIALS

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In the work, when the viscosity of the contacting medium is taken into account, the Rayleigh-Taylor instability is considered. The viscosity of such media was taken into account earlier in [1], which was cited in the monograph [2].
However, an analysis of the equations describing this instability showed that the dependence of the solutions on the vertical coordinate is determined not by the sum of two exponents, but by one of them. This exponent satisfies the Laplace equation for the potential of the velocity. An analysis of the solution associated with the second exponent showed that it does not satisfy the Laplace equation for the potential of the velocity, and represents an unnecessary solution. Therefore, this exponent cannot be taken into account at solving the task. The instability in viscous media is possible when one exponential is taken into account for the case a denser liquid is on top it is shown. In this case, the nature of the instability changes to dissipative, when the growth rate of the instability decreases with increasing viscosity of the media, and the maximum increment is shifted to the region of long-wave perturbations.
On the basis of Rayleigh-Taylor's dissipative instability, the process of electro welding of biological materials is described. The boundary of the joining of biomaterials have a corrugated surface is shown. Estimations of the period and depth of corrugation of the welding surface are made.

References

[1] W.J. Harrison, *Proc. London Math. Soc.*, **6**, 396 - 405 (1908).
[2] S. Chandrasekhar, *Oxford*, 655 p. (1961).

2-11.P

DOCKING 2'-5'OLIGORIBOADENILATES TO DNA-METHYLTRANSPHERASE ECORI

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Disturbance in the balance of methylation of DNA, which in turn serves as a key event in epigenetic deregulation in carcinogenesis, was studied. At the moment, a number of inhibitors of DNA-methyltransferases are known, but their mutagenic and toxic effects are a significant disadvantage of these compounds. Natural and synthetic oligoadenylates, which can bind and affect the work of epigenetic regulators and transcriptional proteins through interaction with regulatory domains, can be used as safe analogues [1].

Docking simulations were run at AutoDock Vina. All calculations were carried out on flexible ligands and a modeled fixed-structure DNA-methyltransferase and with a flexible side chain.

In the course of the research, it was found that binding energies for the natural of 3'-5'A_3 were -5.8 and -5.7 kJ/mol for a rigid and flexible receptor model, respectively. On the other hand, the values of binding energies -8.0 and -7.5 kJ/mole were respectively obtained in the natural 2'-5'A_3. For the epoxy-ribose derivatives of the 2'-5'A_3epoxy, the binding energies values were -5.2 and -5.0 kJ/mol and the amino-adenosine derivative 2'-5'A_3amino -6.7 and -7.3 kJ/mol, respectively. In turn, for the 2'-5'A_3cord, the values were -7.8 and -8.6 kJ/mol. In this case, the binding energy of the cordycypin derivative to the protein is significantly higher in comparison to other oligoribonucleotides. The number of hydrogen bonds varied: when EcoRI was coupled with 2'-5'A_3amino and 2'-5'A_3cord – one hydrogen bond was formed, with 2'-5'-A_3 and 3'-5-A_3 – two, and from 2'-5'-A_3epoxy – 4.

Thus, the analysis of molecular docking suggests that the oligoriboadenilates possess the highest energy of binding with the model DNA-methyltransferase EcoRI.

References

[1] Z. Yu. Tkachuk, *Bipolymers and cell*, **29**, 266-276 (2013).

Section 3. Properties of Classical Liquids: Atomic, Molecular, Ionic and Ionic-electronic Liquids (Molten Salts and Metals)

Oral session

3-1.O

SYNTHESYS OF POLY(IONIC LIQUID)S OF LINEAR AND HYPERBRANCHED ARCHITECTURE CONTAINING THERMALLY RESPONSIVE MACROCATIONS

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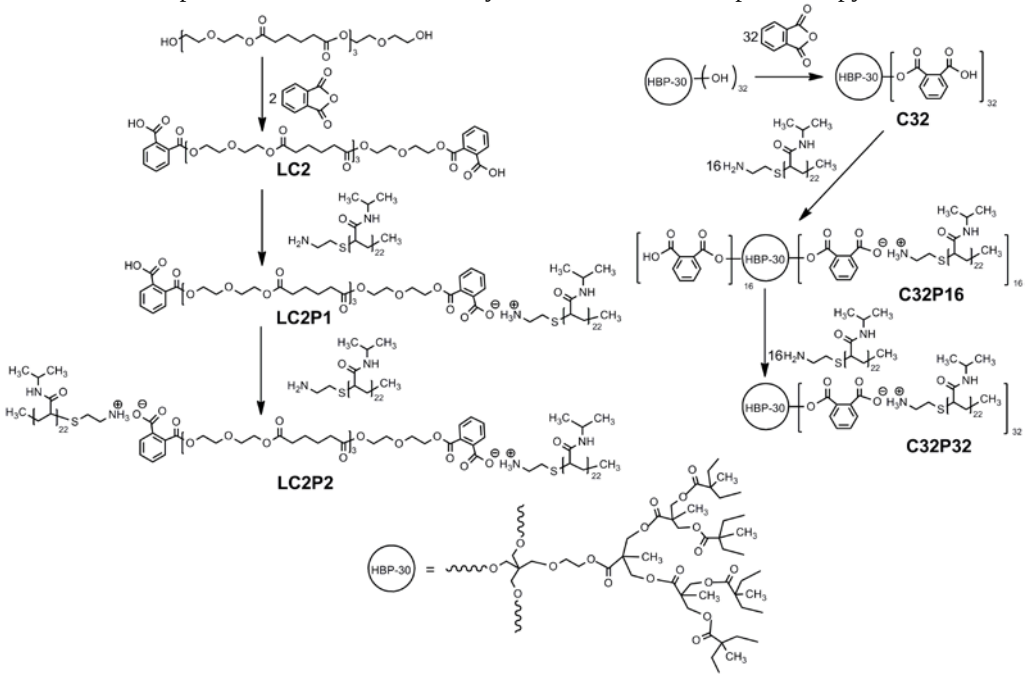
Oligomeric ionic liquids (OILs) and their polymer analogues (PILs) are a new types of polyelectrolytes that combine the unique properties of ionic liquids (IL) and polymers [1,2]. A promising direction in the development of the synthesis of compounds of this type is the providing ion-liquid groups a certain physical function including sensitivity to various physical factors [1,3]. This approach expands the possibilities of molecular design of the compounds and provides the ability to regulate their specific properties, in particular the ability to self-assembly by changing certain physical factors. In this paper we propose the methods for the synthesis of protic anionic linear OILs and hyperbranched PILs with the thermo-responsive macrocations in their composition which change their hydrophilic-hydrophobic properties under the influence of temperature. The ability of these compounds to form a hierarchical structures in condensed state, solutions and on the interfacial water/air surface was studied. The main characteristics of the hierarchical structures and dependence of that characteristics on temperature and molecular architecture of the compounds were determined. The synthesis of the developed OILs and PILs was based on exhaustive acylation of oligo(di(ethyleneglycol)adipate) MM 800 g/mol (in the case of linear OILs LC2P1 and LC2P2) or hyperbranched oligoesterpolyol (in the case of hyperbranched PILs C32P16 and C32P32) containing 32 terminal hydroxyl groups with phthalic anhydride followed by partial (50%) or full neutralization of the resultant carboxylic derivatives by oligo(N-isopropylacrylamide) MM 2500 g/mol containing terminal amino groups (Scheme). Oligo(N-isopropylacrylamide) was characterized by LCST in water solution 30-35^{o}C. These compounds were characterized by FT-IR and ^{1}H NMR spectroscopy.



New poly(ionic liquid)s characterized by simplicity of synthesis and flexible thermal properties. Their glass transition temperature can be tailored from 54 to 77 °C for linear and from 94 to 99 °C for hyperbranched PILs by variation content of peripheral ionic liquid groups. Moreover, we find that PILs form spherical micellar assemblies in aqueous media with size 10-400 nm that depending on PILs architecture [4]. In addition, we observed that molecular mean

square area for the linear oligomeric acid LC2 and OILs based on it at the boundary water / air was in the range 1-12 nm^2, whereas the same values for their hyperbranched analogues were in the range 10-200 nm^2.

References

[1] W. Xu, P.A. Ledin, V.V. Shevchenko, V.V. Tsukruk, *ACS Appl. Mater. Interfaces.* **7**, 12570-12596 (2015).
[2] V.F. Korolovych, P.A. Ledin, A.V. Stryutsky, V.V. Shevchenko, O.A. Sobko, W. Xu, L.A. Bulavin, V.V. Tsukruk, *Macromolecules*, **49**, 8697-8710 (2016).
[3] D. Wang, Y. Jin, X. Zhu, D. Yan, *Progr. Polymer. Sci.*, **64**, 114-153 (2017).
[4] V.F. Korolovych, A.J. Erwin, A. Stryutsky, E.K. Mikan, V.V. Shevchenko, V.V. Tsukruk, *Bulletin of the Chemical Society of Japan*, **90**, 919-23 (2017).

3-2.O

TRANSLATIONAL AND ROTATIONAL DIFFUSION OF IMIDAZOLIUM BASED IONIC LIQUIDS IN ACETONITRILE

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Room-temperature ionic liquids (RTILs) possess a set of remarkable properties for wide industrial applications. In case of electrochemical application of the RTILs the diversity of credible systems can also be expanded by combining RTILs with common electrochemical solvents like acetonitrile (AN).
With the aim to elucidate the rotational and translational diffusive motions of 1-butyl-3-methyl-imidazolium $[Bmim]^+$ cation in RTILs [Bmim][PF_6] and [Bmim][TfO], and their solutions in acetonitrile-D_3 (AN), QENS measurements were carried out as a function of composition: x[Bmim][PF_6] + (1-x)CD_3CN, and x[Bmim][TfO] + (1-x)CD_3CN, where x = 0, 0.01, 0.15, 0.5 and 1. Additionally, the samples with hydrogenated acetonitrile (i) BmimTfO(50%) + CH_3CN(50%) , (ii) BmimPF_6(50%) + CH_3CN(50%), and (iii) pure CH_3CN were also investigated. The experiment was carried out on the OSIRIS time-of-flight spectrometer at ISIS, RAL, UK. Pure RTILs were studied at 298 and 333 K, while solutions were measured at 278, 298 and 333 K.
The dynamic information revealed from the mentioned above measurements in conjunction with the results from NMR spectroscopy [1] and molecular dynamics (MD) simulations already obtained by us, enabled an in-depth analysis of the influence of solvation and association phenomena involved in controlling the properties of RTILs and their mixtures with molecular liquids for their practical applications.

References

[1] B. Marekha, O.N. Kalugin, M. Bria, R. Buchner, A. Idrissi, *J. Phys. Chem. B*, **118,** 5509 – 5517 (2014).

3-3.O

ON THE DEFINITIONS OF THE HYDRODYNAMIC REDUCED DESCRIPTION PARAMETERS BASED ON A NONLOCAL COLLISION INTEGRAL

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We consider a one-component gas with small potential interaction. The investigation is based on the kinetic equation in the case of small interaction [1] with a nonlocal collision integral. In the local approximation this collision integral is the Landau–Vlasov collision integral. The aim of the work is to build the system hydrodynamics on the basis of the nonlocal collision integral.
The hydrodynamic reduced description parameters (RDPs) are the densities of the conserved quantities. In paper [2] it is shown that although the system kinetic energy is conserved in the local approximation, it is not conserved on the basis of the nonlocal collision integral. The system particle density, momentum and total energy are conserved on the basis of the nonlocal collision integral and they are proposed as the system RDPs.
The definitions of the RDPs in terms of the distribution function are obtained on the basis of the expressions for the equilibrium RDPs given in [3]. These definitions are the additional conditions to the kinetic equation. It is shown that in the leading-in-gradients order the Maxwellian distribution function satisfies both the kinetic equation and the additional conditions. Our future plan is to build the system hydrodynamics in the linear-in-gradients order.

References

[1] A.I. Akhiezer and S.V. Peletminsky, Methods of Statistical Physics, Oxford, Pergamon Press, 1981, 376 p.
[2] V.N Gorev and A.I. Sokolovsky, Vìsnik Dnìpropetrovs'kogo unìversitetu. Serìâ Fìzika, Radìoelektronika, **25**, 14 (2017).
[3] Yu. L. Klimontovich, Statistical Physics, Moscow, URSS, 2014, 608p (in Russian)

3-4.O

ION ASSOCIATION AND SOLVATION IN THE SOLUTIONS OF IMIDAZOLIUM-BASED ROOM TEMPERATURE IONIC LIQUIDS IN PROPYLENE CARBONATE

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Nowadays room temperature ionic liquids (RTILs) in mixture with molecular liquids are successfully used as electrolyte solutions for different chemical power sources [1]. Detailed understanding of ion association and solvation at the microscopic level gives one an unique opportunity to predict macroscopic properties of such systems.
In presented work seven RTILs (1-ethyl-3-methylimidazolium, 1-hexyl-3-methylimidazolium, 1-butyl-4-methylpyridinium tetrafluoroborates and 1-butyl-3-methylimidazolium trifluoromethanesulfonate, tetrafluoroborate, hexafluorophosphate and bromide) in mixture with propylene carbonate (PC) were studied by conductometry in diluted concentration region within the temperature range 278.15 − 388.15 K. Moreover, 1-butyl-3-methylimidazolium tetrafluoroborate, hexafluorophosphate and bromide were also studied by densimetry at different temperatures.
The limiting molar conductivities and association constants were derived using the Lee–Wheaton equation from a conductometry data. Investigated RTILs in PC demonstrate low association with slightly larger constant for 1-butyl-3-methylimidazolium bromide. Association constant increase a little with temperature increase and is more influenced by anion size and nature then of cation of RTIL. Limiting molar conductivities of RTILs with the same anion decrease with the increase of alkyl chain of cation. Additionally, detailed analysis of partial molar volumes of the investigated RTILs was performed. The ionic molar volumes at infinite dilution were compared with structural volumes of ions from quantum chemical calculations in order to investigate solvation effects.

References

[1] Hongtao Liu, Yang Liu and Jinghong Li, *Phys. Chem. Chem. Phys.*, **12**, 1685–1697 (2010).

3-5.O

SPECIFIC FEATURES OF STRUCTURE AND DYNAMICS OF LIQUID METALS AT HIGH PRESSURES

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Liquid metals under high pressure show specific short-range order in structure [1,2] and emergence of unusual high-frequency transverse modes in collective dynamics [3]. These features are connected to the partial localization of electrons in the interstitial regions [1,2]. Recently similar dynamic features in collective dynamics were reported for liquid Tl [4]. We will present new results obtained by means of *ab initio* molecular dynamics simulations for liquid Pb and Si, as well as for a binary metallic melt Ga-Sb. We will discuss changes with pressure in a specific for liquids "positive dispersion" of acoustic excitations and propagation gap for transverse excitations. We will also discuss a problem of metallization of Hydrogen fluid at high temperature with a special focus on electron-ion correlations in the vicinity of the transition from molecular to atomic fluid Hydrogen under pressure.

References

[1] T. Bryk *et al*, *Phys. Rev. Lett.*, **111**, 077801 (2013).
[2] T. Bryk, I. Klevets, G. Ruocco, T. Scopigno, A.P. Seitsonen, *Phys. Rev. B*, **90**, 014202 (2014).
[3] T. Bryk, G. Ruocco, T. Scopigno, A.P. Seitsonen, *J. Chem. Phys.*, **143**, 104502 (2015).
[4] T. Bryk, T.Demchuk, N.Jakse, J.-F.Wax, *Frontiers Phys.*, **6**, 6:1-8 (2018).

3-6.O

INFLUENCE OF NANOPARTICLES ON THERMOPHYSICAL PROPERTIES OF Sn–Ag–Cu ALLOYS

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The alloys based on ternary Sn–Ag–Cu system are considered as the most promising materials for lead-free solders due to their excellent physical and mechanical properties. But employing of near-eutectic Sn–Ag–Cu alloys in soldering process connects with some disadvantages comparing to conventional Pb-Sn alloys, such as higher melting points and poor mechanical shock resistance. Thus, a number of studies were related to improvement of the physico-chemical and mechanical properties of Sn–Ag–Cu-based solders introducing additional different nano-sized components. In this work, two types of nanosized admixtures, namely, carbon nanotubes (CNT) and bimetallic nano admixtures CoPd were added to the basic $Sn_{96.5}Ag_3Cu_{0.5}$ (SAC305) alloys. Thermophysical and mechanical properties of SAC305 alloys with these nanosized admixtures were investigated over a wide temperature range.

METALLIC HYDROGEN AS AN ALKALINE METAL

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We have calculated the coefficients of electrical resistivity and thermoelectric power, temperature resistivity coefficient, free energy, entropy, and the equation of the state of liquid metallic hydrogen in a wide range of densities and temperatures. All calculations were carried out in the framework of perturbation theory for electron-proton interaction. The electrical resistivity was calculated in the second and third order perturbation theory, all thermodynamic functions in the zero, second and third order. Since the electron-proton interaction for hydrogen is known exactly, then there is the possibility to perform all calculations without the use of fitting parameters. This does not mean that the only source of error is the use of perturbation theory. When we are considering the degenerate electron gas, there is a need for another fundamental approximation - the local field approximation with respect to the potential of the exchange interaction and the correlations of conduction electrons. When we are considering the proton subsystem, there is a need to use the model of solid spheres. Two parameters of this model for simple metals - the diameter of solids sphere and the packing fraction coefficient can be found from the analysis of experimental data on neutron scattering. For all the simple metals, this analysis is performed only at one point, namely for the melting temperatures of these metals. For liquid metallic hydrogen, even such data are missing. Therefore, the solid spheres diameter we were looking for from the analysis of a pair of effective proton-proton interaction. To calculate this one, we used the perturbation theory by electron-proton interaction in the second and third orders. This approach allowed to simulate the density and temperature dependence of the hard sphere diameter and the packing fraction coefficient in a wide range of temperatures and densities. For declared by the authors of the discovery of metal hydrogen temperatures and densities of our calculated pressure values are quite satisfactorily consistent with those obtained experimentally. The consistency of the theoretical and experimental values of the electrical resistance was much worse.

In order to further test the reliability of the results obtained for liquid metallic hydrogen, we have calculated the corresponding characteristics of liquid alkali metals Li and Na in similar approximations and in the same range of temperatures and densities. The dependence of all calculated characteristics of liquid metal hydrogen, lithium and sodium was similar, and for Li and Na they were quantitatively well-coordinated with known experimental data for melting temperatures. Interestingly, for Li and Na, the packing fraction coefficient achieved at the melting point is the same. We took this value as a fitting parameter for liquid metal hydrogen. In the result, we calculated the value of the pressure of metallic hydrogen almost perfectly coincided with the experimentally obtained, and the electrical resistivity we calculated was significantly closer to that obtained experimentally. Consequently, the view of liquid metallic hydrogen as an ordinary alkaline metal was surprisingly productive.

3-8.O

LOCAL ATOMIC ORDER IN AL-GE-FE(NI) MELTS WITH LOW CONTENT OF TRANSITION ELEMENT

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Al-bases alloys with addition of iron and nickel have different applications due to combination of low density and high corrosion resistance, elasticity and mechanical strength. One of the most promising cost-effective joining techniques of these alloys is diffusion brazing. The brazing materials should possess lower melting points than the substrates. The structure similarity between phases formed in the joint area and substrates is required. Crystalline germanium meet first requirement but phase formation from liquid state is still not clear. The Al-Ge-Fe and Al-Ge-Ni ternary diagrams are characterized by wide glass-forming region after rapid solidification that opens good opportunities in producing new materials through subsequent crystallization.

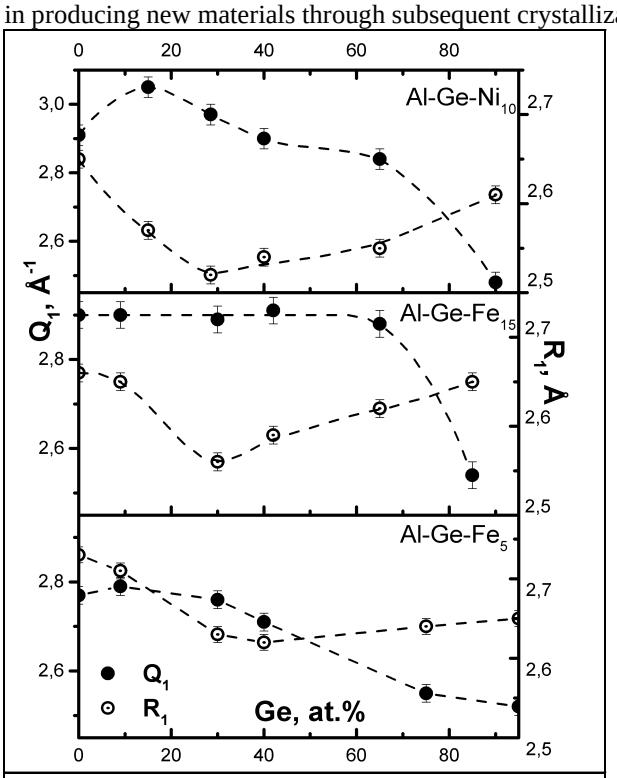

Figure 1. Structure parameters of Al-Ge-Fe and Al-Ge-Ni melts at 1000°C.

We have studied ternary melts with overall composition Al-Ge-Fe_5, Al-Ge-Fe_5, and Al-Ge-Ni_{10} by means of X-ray diffraction method at 1000°C and 1500°C. Positions of the first maximums on the structure factors (Q_1) and pair distribution functions (R_1) are presented on the Fig.1. As one can see, increase in Fe content leads to higher values of Q_1 and simultaneous decrease of the nearest interatomic distance. Al-Ge-Ni_{10} melts have relatively high values of Q_1 and lower values of R_1 comparing to Al-Ge-Fe ternary melts due to stronger interactions in Al-Ge-Ni_{10}. Given tendencies are confirmed by more negative values of the enthalpies of mixing in Al-Ni melts than in Al-Fe melts [1]. An increase of temperature of the melts up to 1500°C leads to the slightly lower values of Q_1 and higher values of R_1.

Structure models of the investigated melts have been obtained by Reverse Monte Carlo simulations and analyzed by Voronoi-Delaunay diagrams. It was found that dense non-crystal atomic packing is decreasing with increase in Ge content in the melts.

References

[1] P. Desai *J.Phys. Chem. Ref. Data*, **16,** 109-124 (1987).

3-9.O

STRUCTURE-SENSITIVE PROPERTIES OF HIGH-ENTROPY ALLOYS

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Conventional alloys are mainly based on one principal element with different kinds of alloying elements added to improve their properties. These alloys form an alloy family based on the chosen principal element. However, the number of elements in the periodic table is limited, thus the alloy families, which can be developed, are also limited. The new concept, first proposed in 1995, has been named a high-entropy alloy. According to proposed definition, any multi-component alloy consisting of five or more principal elements, which have a concentration between 5 and 35 at.%, belongs to the high-entropy alloy family. Besides principal elements, HEAs could contain also minor elements with concentrations below 5 at.%. The main goal of the present study was to receive a set of reliable thermophysical data of the liquid phase of selected high-entropy alloys. The multicomponent high-entropy alloys containing Al, Bi, In, Co, Cu, Fe, Ni and their sub-system alloys with equiatomic compositions were chosen for the present research.

3-10.O

ON THE DEPENDENCE OF THE PLASMA HEAT CONDUCTIVITY ON THE TEMPERATURE

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The completely ionized plasma is considered in the generalized Lorentz model. The research is based on Landau kinetic equation. The interactions of ions with each other and the electrons with each other are neglected; the subsystem of ions is considered to be equilibrium and has temperature T_0. The kinetic equation has the form in this model:

$$\frac{\partial \mathrm{f}_p(x,t)}{\partial t} = -\frac{p_n}{m}\frac{\partial \mathrm{f}_p(x,t)}{\partial x_n} + eE_n(x)\frac{\partial \mathrm{f}_p(x,t)}{\partial p_n} + \hat{K}\mathrm{f}_p(x,t), \tag{1}$$

where $\hat{M}$ is linear operator of the collision integral. The standard definitions of the density n of temperature T and mass velocity υ_l of the electron subsystem [1] is used, so we obtain time equations

$$\frac{\partial n}{\partial t} = -\frac{\partial n\upsilon_l}{\partial x_l}, \qquad \frac{\partial \upsilon_l}{\partial t} = \frac{1}{n}\upsilon_l\frac{\partial n\upsilon_m}{\partial x_m} - \frac{1}{mn}\frac{\partial t_{lm}}{\partial x_m} + \frac{1}{mn}\left(\int d^3 p p_l \hat{M}\mathrm{f}_p - enE_l\right),$$

$$\frac{\partial T}{\partial t} = \frac{3T - m\upsilon^2}{3n}\frac{\partial n\upsilon_l}{\partial x_l} + \frac{2}{3n}\frac{\partial t_{lm}}{\partial x_m}\upsilon_l - \frac{2}{3n}\frac{\partial q_l}{\partial x_l} + \frac{2}{3n}\int d^3 p(\varepsilon_p - p_l\upsilon_l)\hat{M}\mathrm{f}_p \tag{2}$$

($\varepsilon_p \equiv p^2/2m$). These equations are the hydrodynamics equations of the subsystem of electrons with account for relaxation processes $T - T_0 \to 0$, $\upsilon_l \to 0$, that allows us to introduce a small parameter μ. The solution of the kinetic equation is sought in the form of depending on functions $\xi_\mu(x)$: $n(x)$, $\upsilon_l(x)$, $T(x)$ functional $\mathrm{f}_p(x,\xi)$ in perturbation theory in their gradients

$$\mathrm{f}_p = w_p\left(1 + g_p + C_{lp}E_l + D_{lp}\frac{\partial \ln n}{\partial x_l} + G_{lp}\frac{\partial T}{\partial x_l} + F_{slp}\frac{\partial \upsilon_s}{\partial x_l} + O(g^2)\right), \qquad w_p \equiv \frac{n}{(2\pi m T_0)^{3/2}}e^{-\frac{\varepsilon_p}{T_0}} \tag{3}$$

($\hat{M}w_p = 0$, g is parameter of smallness of gradients and field). The equations for functions g_p, C_{lp}, D_{lp}, G_{lp}, F_{lp} are derived and investigated in perturbation theory in μ. The most difficult for an approximate solution is the equation obtained for g_p

$$a_l\partial g_p/\partial\upsilon_l + b\partial g_p/\partial T = \hat{K}g_p \tag{4}$$

($\hat{M}w_p h_p \equiv -w_p\hat{K}h_p$ is true for an arbitrary function h_p). The coefficients a_l, b are determined from the additional conditions that follows from definitions of the parameters $\xi_\mu(x)$. As a result the dependence of the plasma heat conductivity on temperature T and velocity υ_l was found.

References

[1] Akhiezer A.I. and Peletminskii S.V. Methods of Statistical Physics. Oxford: Pergamon Press. (1981).

3-1.P

THERMOPHYSICAL PROPERTIES OF LIQUID BINARY NaF-LaF_3, NaF-NdF_3 AND TERNARY NaF–LiF–LaF_3, NaF–LiF–NdF_3 EUTECTIC ALLOYS

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Thermophysical properties (electrical conductivity, thermoelectric power and viscosity) of liquid binary NaF-LaF3, NaF-NdF3 and ternary NaF–LiF–LaF3, NaF–LiF–NdF3 systems were investigated in the wide temperature intervals above the melting points. It was revealed that the alloy composition has a significant influence on the interval of melt homogeneity and behaviour of the thermoelectric power temperature coefficient. It was found that a small shift from the peritectic to eutectic composition increases considerable the viscosity. A correlation between the structure and thermophysical properties has been analyzed. It is shown that the ionic liquid heterogeneous system NaF-LaF3 becomes a homogeneous ionic solution at a temperature, which exceeds the melting temperature of more than 130 K, and the heterogeneous ionic liquid system NaF-NdF3 becomes ionic solution at a temperature higher than the melting point of about 150 K, which is consistent with the XRD results. A comparison of the physical properties of the investigated systems with their ternary analogs formed by adding LiF to the original binary systems was described. It was revealed that addition of the LiF does not change the temperature dependence of the viscosity of the corresponding ionic liquid systems, but increases their conductivity by a factor of 1.5. The results can be used in modelling a blanket for the liquid salt reactors of new generation.

INTERRELATION OF VIBRATIONAL RESONANCES AND PHONON DISPERSION IN LIQUID BENZENE

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A characteristic feature of benzene is the sequence of coupled vibrational resonances (VR). The basic VRs are R_1 **(ν_1 + ν_6, ν_8)** and R_2 **(ν_{20},** R1 + **ν_{19})** connected to the closeness of the frequencies **$\nu_1 + \nu_6 \approx \nu_8$, ($\nu_1 + \nu_6$) + $\nu_{19} \approx \nu_8 + \nu_{19} \approx \nu_{20}$**. By combining RP R1,2 with other oscillations, for example R_2 **(ν_{20}, $R_1 + \nu_{19}$) ± ν_6**, a large set of Raman scattering (RS) is formed, which overlap and become more complicated (see Fig. 1a). By comparing the quantum-chemical calculations (B3LYP, 6-311G (d, p), 6-311 ++ G (d, p)) for the $^{12}C_6H_6$, $^{13}C^{12}C_5H_6$ molecules with experimental data, the frequency of a number of "silent" oscillations, for example, **ν_{13}** = 3033 cm^{-1}, as well as the frequencies in the RS $R_{1,2}$. The key role here is played by the analysis of the half-widths **$\delta\nu$** of individual components of the Raman spectrum and their anharmonic shifts **$\Delta\nu_A$**, rather than the intensity ratio, as illustrated in Fig. 1a. In the RS $R_{2\text{-}\nu6}$ and in the IR spectrum, the more intense high-frequency component **(ν_8 + ν_{19}) -ν_6,** although in RS the R_1 low-frequency component $\nu_1 + \nu_6$ (the inset in Fig. 1a), but it has a large half-width $\delta\nu$. And in the RS $R_{2\text{-}\nu6}$ for the component with the main tone ν_8 **$\Delta\nu_A$** = -0.7 cm-1, and for **[(ν_1 + ν_6) + ν_{19}] -ν_6 $\Delta\nu_A$** = -13.5 cm^{-1}. Analysis of the values of **$\delta\nu$** and **$\Delta\nu_A$** allowed to make correct identification of frequencies for the set of Raman spectra.

Most of the vibrational bands (VB) of liquid benzene are multiplets, which until now had no physical explanation. Therefore, for the set of observed VB only ~ 1/3 of the components are interpreted. Taking into account that the vibrational modes in liquids have collective properties and are characterized by the wave vector **k [1,2]**, we have done a great deal of work on the coordinated classification of the set of additional components. We associate them with the existence of quasiphonon branches **ν (k),** whose definite states manifest themselves in the vibrational spectra as a result of disordering of the liquid structure. A comparison of the theoretical and experimental values for the phonon branches **ν_8 (k)** and **(ν_1 + ν_6) (k)** of liquid benzene is shown in Fig. 1b. Here, the integer parameter **m**, numbering the components of the vibrational multiplets, is proportional to **k**. It can be seen that resonant splitting of frequencies in the region of large values of **k** is greater than for **k**≈0. The inset in Fig. 1b shows the change in the observed intensities of various components of the multiplets **ν_8, ν_1 + ν_6**. It can be seen that the ratio IR of the intensities of the Raman components can vary substantially, which is confirmed by the data in Fig. 1a.

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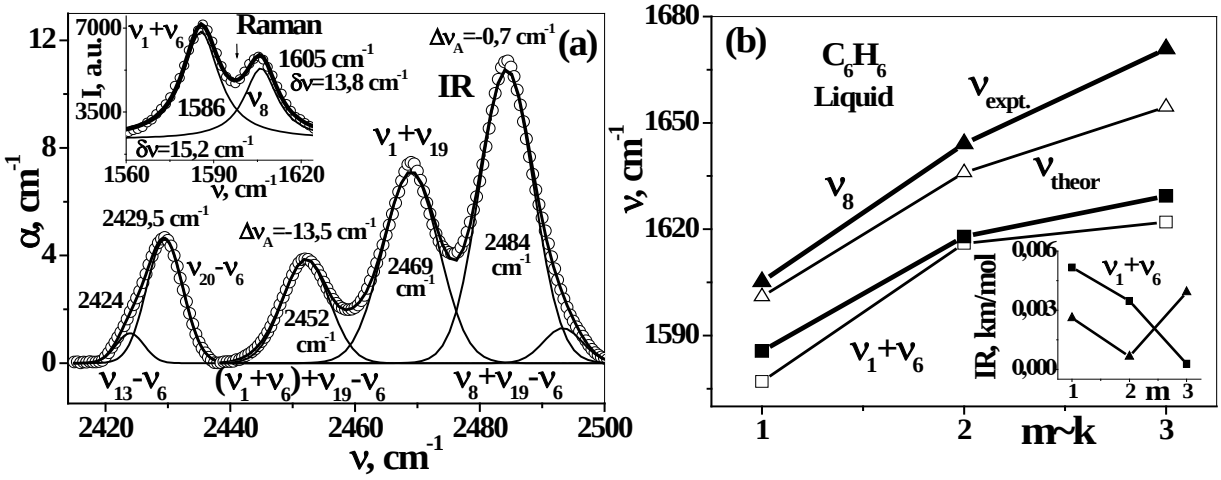

3-3.P

PHASE-FORMATION PROCESSES IN AMORPHOUS ALLOYS BASED ON Fe, Ni And Co UNDER THE INFLUENCE OF THERMAL TREATMENT

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Modern thermodynamically nonequilibrium materials with amorphous structure are characterized by a number of unique physicochemical properties. An actual direction of research of metallic glasses is the development of methods to achieve nanostructured state by partial crystallization of amorphous alloys due to external influences. Such influences include heat treatment (the isothermal and non-isothermal annealing at temperatures below than temperature of crystallization, thermocycling, cryotreatment); intensive plastic deformation; irradiation by particles of various nature. Large attention to heat treatment of alloys with the amorphous structure is explained by an acquisition of the special properties in the nanocrystalline state. In the series of experiments on amorphous alloys heat treatment aiming to increase the thermal stability of alloys and developing the ways to obtain alloys in the nanostructural state as well as investigating mechanical properties of nanostructural materials were conducted.

Based on our analysis of results from calculations within the high-temperature stability of amorphous alloys theory [1], two areas of its practical application were proposed: enhancing the thermal stability of amorphous alloys by isothermal annealing in the range of temperatures where crystalline nuclei can transform into the amorphous phase and transforming the amorphous state into a nanocrystalline state via prolonged low-temperature isothermal annealing. It was confirmed experimentally that external effects which reduce the difference between the chemical potentials of the *i*-th component in an amorphous matrix and in frozen-in crystallization centers (in the temperature region where $\Delta\mu_i < 0$) result in the dissolution of frozen-in crystallization centers and thus to an increase in the thermal stability of amorphous alloy. Prolonged low-temperature isothermal annealing allows us to form nanostructured states. The purification of an amorphous matrix of frozen-in crystallization centers was theoretically verified and experimentally achieved by analyzing the theses of the thermodynamic theory of the high temperature stability of amorphous alloys, which state that there exists a range of temperatures that corresponds to fulfillment of the condition of the dissolution of frozen-in crystallization centers. It was shown that the proposed regimes of thermal treatment allow us to expand the ranges of the thermal stability of amorphous alloys based on iron by 20–40 K. The value of microhardness then falls by 16–21%, indirectly proving the reduction of the crystalline phase part in the samples. The increased thermal stability of the investigated multicomponent amorphous alloys can be explained by the amorphous matrix being purified of frozen-in crystallization centers, as was confirmed by the results from electronmicroscopic investigations.

Based on the analysis of high-temperature thermodynamic stability of amorphous alloys theory proposed a method for producing amorphous-nanocrystalline state from the initial amorphous. The empirically determined temperatures of isothermal annealing (at which the subsequent thermal treatment of the initial samples was carried out) are presented in Table . At the determined annealing temperatures, thermal processing of the initial amorphous alloys was carried out for 1 hour and the volume part of the crystalline phase formed during the annealing was calculated. As a parameter for comparing the mechanical properties of metallic glasses in the initial state and alloys after the heat treatment, the value of the microhardness *H* was used. The results of the microhardness measurements carried out are presented in Table.

Table . Temperatures T_k of the onset of intense crystallization for the initial alloys, temperatures T_k of preliminary thermal treatment and volume part of crystalline phase X after thermal treatment at temperature T_k" and relative change of microhardness

Amorphous alloy	T_k, K	T_k", K	*X*	$(H_{annearling} - H_0) / H_0$,%
$Fe_{80}B_{14}Si_6$	770	750	0,16	17,9
$Fe_{40}Ni_{40}B_{20}$	710	685	0,22	18,8
$Ni_{78}B_{18}Si_4$	730	705	0,19	20,8
$Co_{67}Fe_3Cr_3Si_{15}B_{12}$	458	420	0,17	15,7
$Co_{55}Fe_5Ni_{14}Si_{16}B_{10}$	529	500	0,20	14,6

The alloys in the amorphous-nanocrystalline state were made, as evidenced by the results of electronmicroscopic studies. It was found that the microhardness of the obtained materials is increased as compared to the amorphous state to initial due to an increase of the frozen-in crystallization centers size and the formation of amorphous-nanocrystalline state.

3-4.P

CALCULATION OF SHEAR AND BULK ELASTIC MODULES OF AQUEOUS SOLUTIONS OF ELECTROLYTES TAKING INTO ACCOUNT THE GENERALIZED INTERACTION POTENTIAL FOR ION-MOLECULAR SYSTEMS

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To study the structure of liquids and solutions, transport phenomena and mechanism of relaxation processes occurring in them, subject of many theoretical and experimental works. Important information about the kinetics of irreversible processes in electrolyte solutions give the coefficients of shear η_S and η_V bulk viscosity, and shear μ and bulk *K* modules of elasticity.

In [1,2] obtained an expression for bulk *K* and shear μ elastic moduli, which are determined by the potential energy of the interaction $\Phi_{ab}(|\vec{r}|)$ and the radial distribution function $g_{ab}(|\vec{r}|)$. In [2,3], at the optimal choice $\Phi_{ab}(|\vec{r}|)$ and $g_{ab}(|\vec{r}|)$ numerical calculations of these coefficients for aqueous solutions of NaCl in approximation theory Macmillan-Mayer. The contribution of the solvent in the μ and *K* modules of elasticity is taken into account through the ratio of the dielectric constant of the solvent ε_{ss}, as well as coefficients of friction β_a and β_b the ions of the sorts *a* and *b*. However, in real models of electrolyte solutions between the structural units have ion-dipole and dipole-dipole interaction.

The purpose of the communication is the realization of numerical calculations for shear μ and bulk *K* modules of elasticity were obtained in [3,4] taking into the most complete account of ion-ion $\Phi^0_{ab}(r)$, ion-molecular $U_{is}(r)$ and intermolecular $U_{ss}(r)$ interactions, the potential of which is as follows:

$$\Phi_{ab}(r,\vartheta) = \Phi^0_{ab}(r) + \left(U_{is}(r) + U_{ss}(r)\right)\cos\vartheta, \qquad (1)$$

where $\Phi^0_{ab}(r) = 4\varepsilon_{ab}\left(r^{-12} - r^{-6}\right) + \frac{fz_az_be^2}{kT\varepsilon_{SS}d_{ab}}\frac{\exp(\chi^*)}{1+\chi^*}\frac{e^{-\chi^* r}}{r}$, $U_{is}(r) = \frac{f(z_a+z_b)e\mu}{d^2_{ab}}\frac{1}{r^2}$, $U_{ss}(r) = -\frac{f\mu^2}{d^3_{ab}r^3}$,

$\varepsilon_{ab} = \sqrt{\varepsilon_{aa}\varepsilon_{bb}}$, $d_{ab} = (d_a + d_b)/2$ - are parameters of the potential Lennard-Jones, $r = r_{ab}/d_{ab}$ - unite mutual distance, $f = (4\pi\varepsilon_0)^{-1} = 9\cdot10^9$ м/Ф, ε_0 - the electric constant, ε_{SS} -is the dielectric coefficient of the solvent, *e*- is the elementary charge, z_a, z_b -is the valence of ions of the sorts *a* and *b*, μ-dipole moment, $\chi^* = d_{ab}\chi_a$ - given the inverse Debye radius of shielding $\chi^2 = \sum_a n_a e_a^2/\varepsilon_{SS}\varepsilon_0 kT$.

The expression for the radial distribution function $g_{ab}(r,\vartheta)$ taking into account (1) adopted in the form [3,4]:

$$g_{ab}(r,\vartheta) = y(\rho^*)\exp(-\Phi_{ab}(r,\vartheta)/kT) = g^0_{ab}(r)\exp[-\left(U_{is}(r) + U_{ss}(r)\right)\cos\vartheta/kT] \qquad (2)$$

where $g^0_{ab}(r) = y(\rho^*)\exp(-\Phi^0_{ab}(r)/kT)$, $y(\rho^*) = (2-\rho^*)/2(1-\rho^*)^3$ - the function of a Carnahan-Starling, $\rho^* = \pi n d^3_{ab}/6 = \pi\rho d^3_{ab}N_0/6M$ - unite density, ρ- is the density of the solution, N_0 - is Avogadro's number, *M* - is the molar mass.

On the basis of (1) and (2) numerical calculations of friction coefficients β_1, β_2 and relaxation times τ_1, τ_2, τ_{11}, $\tau_{12} = \tau_{21}$, τ_{22}, as well as elastic moduli μ and *K* used explicit analytical expressions are obtained in [3,4]. The obtained results are in good agreement with the experimental data.

References

[1] S.Odinaev, A.A.Adamov Molecular theory of structural relaxation and transport phenomena in liquids. – Dushanbe: Donish, 1998. -230 p.

[2] S. Odinaev, D.M. Akdodov, N.Sh. Sharifov, Kh. Mirzoaminov, *Russian Journal of Physical Chemistry A*, **84(6)**, 954–959 (2010).

[3] S. Odinaev, D.M. Akdodov, *Reports of the Academy of Sciences of the an Republic Tajikistan*, **58(10)**, 908-915 (2015).

[4] D.M. Akdodov, *News of Academy of Sciences of the Republic of Tajikistan. Department of Physical, Mathematical, Chemical, Geological and Technical Sciences*, **161(4)**,65-74 (2015).

3-5.P

THE STUDY OF DIELECTRIC PROPERTIES OF ELECTROLYTE SOLUTIONS WHEN RELAXING THE FLOW DECAY BY POWER LAW

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Study of physico-chemical parameters of water and water solutions dedicated to the many works and in a large part of them investigated the static value of the dielectric constant. In the presence of external variables electric field, along with the static dielectric coefficient, is the frequency-dependent coefficients of the dielectric constant and dielectric loss. However, the microscopic determination of these coefficients of electrolyte solutions at the present time is very difficult as you must define them in a wide range of frequencies, depending on the thermodynamic state parameters, given the structure of the solution. Optimal use of fluids in all areas of chemical engineering, biology, medicine, etc., requires knowledge of their physic-chemical properties in a wide interval of changes of the state parameters and frequencies. Therefore, it is of interest microscopic determination of the analytical expression of the dynamic coefficients of dielectric constant and dielectric loss depending on the structure of the solution.

On the basis of kinetic equations for one-particle and two-particle distribution functions give dynamic equation for the current density of conductivity. Making a last Fourier transform in time and comparing with the Fourier-image of the Ohm's law for current density conductivity, obtained the analytical expression for the complex dynamic electro conductivity $\tilde{\sigma}(\omega)$. Using the connection between the analytical expressions of the complex coefficient of conductivity $\tilde{\sigma}(\omega)$ and complex dielectric coefficient $\tilde{\varepsilon}(\omega)$ [1], taking into account the contributions of structural relaxation and separating the real and imaginary parts of the latter, for the coefficients of dielectric constant $\varepsilon_1(\omega)$ and dielectric loss $\varepsilon_2(\omega)$ of the obtained analytical expressions, which, along with the friction coefficients and the relaxation times of ions in momentum and configuration space, in expanded terms contain the potential energy of ion-molecular systems and radial distribution function.

For numerical calculations $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ should be the choice of the model solution and the explicit form of the potential energy of ion-molecular systems and radial distribution function.

References

[1] Odinaev S., Makhmadbegov R.S. Studying the frequency dispersion of the dielectric permeability of electrolyte solutions // *Russian Journal of Physical Chemistry A*, **90(1)**, 89-94 (2016).

3-6.P

THE FREQUENCY ASYMPTOTICS FOR THE ELECTROCONDUCTIVITY AND THE MODULUS OF ELECTROELASTICITY SOLUTIONS OF ELECTROLYTES

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Experimental study of the nature of internal relaxation processes in liquids and their solutions, dedicated a lot of work, a detailed review of which is given in [1,2]. Widely analyzed region of frequency dispersion of transport coefficients, elastic and acoustic parameters in the presence of heat, shear and structural relaxation in liquids and relaxation processes (ion, dipole, chemical, etc.) in solutions of electrolytes. Along with studies of these parameters of solutions in a wide range of frequency dispersion, even areas of low and high frequency asymptotics. It is determined that the region of frequency dispersion of transport coefficients, elastic and acoustic parameters is the wide ~10^4 - 10^5 Hz, taking into account the contributions of structural relaxation, and taking into account the contributions of translational relaxation processes in these settings, is a narrow, ~10^2 Hz. The method of molecular dynamics is determined that the kinetic coefficients and acoustic parameters have low frequency asymptotics $\omega^{1/2}$, and the moduli of elasticity – $\omega^{3/2}$. At high frequencies the kinetic coefficients – ω^{-1}, and the elastic moduli do not depend on frequency.

In [3,4] by the method of kinetic equations, received the analytical expressions for the coefficient of conductivity $\sigma(\omega)$ and modulus of electroelasticity $\in(\omega)$ solutions of electrolytes. We studied the frequency dispersion region $\sigma(\omega)$ and $\in(\omega)$ their asymptotic behaviors at low and high frequencies. For and taking into account the contributions of structural relaxation, obtained the same frequency asymptotics at low ($\omega\tau_a << 1$) and high ($\omega\tau_a >> 1$) frequencies, which coincides with the results of molecular dynamics for frequency-dependent asymptotic behavior of the kinetic coefficients and elastic moduli of liquids and their solutions, and taking into account the contributions of relaxation processes, when the flow of damped exponential low and high frequency asymptotics $\sigma(\omega)$ and $\in(\omega)$ coincide with the results of the general relaxation theory [1,2].

References

[1] I. G. Mikhailov, V. A. Solov'ev, and Yu. P. Syrnikov, Principles of Molecular Acoustics. - Nauka, Moscow, 1964, 514 p. [in Russian].

[2] Physical acoustics: Properties of gases, liquids and solutions. Edited by Warren P. Meson. V. 2. Part A. –Moscow. Mir 1968. 487 p. [in Russian].

[3] S.Odinaev, A.A.Adamov *Molecular theory of structural relaxation and transport phenomena in liquids*. – Dushanbe: Donish, 1998. -230 p. [in Russian].

[4] Odinaev S., Idebug H. *Reports of the Academy of Sciences of the an Republic Tajikistan*, **61**, (2018).

3-7.P

ON THE COMPLEX ROUGHNESS FUNCTION OF IMPEDANCE OF HOMOGENEOUS CHEMICAL REACTION OF FIRST ORDER

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The generalized Gerischer impedance theoretical model for a sinusoidal-shaped electrode has been developed. The impedance is presented as an expansion by the small parameter, which is equal to the ratio of the amplitude to period length of surface roughness. For the case of a weak roughness, we have derived the general expression for the complex roughness function and established its limiting behavior (Fig. 1). It is shown that roughness does influence the value of parameters extracted from low - frequency region of an impedance measurement. In the low - frequency range the Gerischer impedance of a rough electrode is kinetically controlled. In anomalous intermediate-frequency region, impedance exhibits frequency dispersion which is caused by the roughness. The roughness function phase angle behavior gives rise to anomalous behavior of the generalized Gerischer impedance phase angle in the intermediate frequency domain. It is shown, that phase angle increases with increasing roughness. Our mathematical model did not provide information on the frequency dispersion associated with CPE behavior. In the frame of the proposed model, at high frequencies, the Warburg type response with phase angle equals to $\pi/4$ is observed. However, for correct description of the influence of electrode geometry in the range of high frequencies calculation of potential in an outer domain is required.

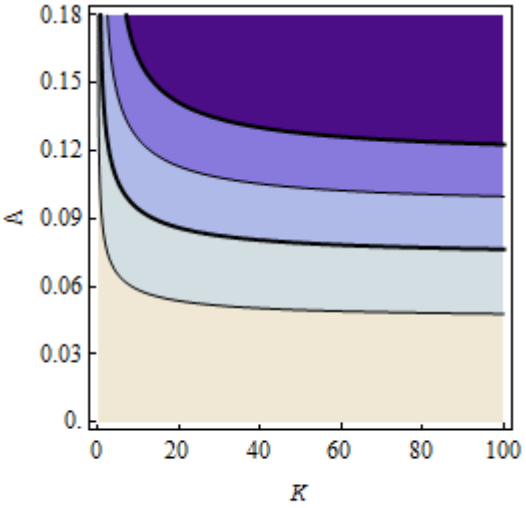

Fig. 1. Contour plots of the roughness function at zero frequency for different values of the control parameters *A* (dimensionless roughness parameter) and *K* (dimensionless effective rate constant of homogeneous preceding chemical reaction)

References

[1] V.V. Pototskaya and O.I. Gichan, *Electrochim. Acta*. **235**, 583–594 (2017).

3-8.P

TEMPERATURE-INDUCED CHANGES OF THE STRUCTURE AND FREE VOLUME OF LIQUID BISMUTH

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In accordance with the generally accepted points of view, the structure of simple liquids varies continuously from the melting to its boiling point. On the other hand, the structure of molten semi-metals, characterizing by the presence of partially covalent bonds in the crystalline state, is described by more complex structure models. Bismuth is the most prominent representative of the semi-metals, which in the crystalline state forms a rhombohedral lattice with a coordination number of 6. In the process of melting, the release of valence electrons occurs, resulting in the compacting of the structure of liquid bismuth. In accordance with modern ideas, the structure of liquid bismuth should be regarded as a combination of “regular” and “irregular” structures, where the term “regular” is used to denote the structure of an ordinary liquid. The “irregular” structure is associated is with a distortion of the structure of the liquid bismuth due to the existence of an excess free volume. However, this process occurs in a wide range of temperatures, and until now is still not fully understood. In this regard, there is a necessity for a more detailed study of the structure of the semimetals, in particular by means the computer simulation methods.
In this work, the investigations of the structure of liquid bismuth were carried out by molecular dynamics simulation method using the EAM potential of interatomic interaction. As a result of the simulation, an analysis of the temperature dependences of the main structure parameters, the free volume and the coordination polyhedra of liquid bismuth in a wide temperature range was carried out.

3-9.P

THERMODYNAMIC AND KINETIC PROPERTIES OF METALLIC NITROGEN AND OXYGEN

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Oxygen and nitrogen are considered as simple liquid metals. For them, the coefficients of electrical resistivity and thermoelectric power, free energy, entropy and equation of state in a wide range of densities and temperatures are calculated. All calculations were carried out in the framework of the perturbation theory for the pseudopotential by electron-ion interaction. The electrical resistivity was calculated in the second and third order of perturbation theory, all the thermodynamic functions in the zero, first, second, and third order. The complexity of the oxygen and nitrogen is that the pseudopotential for these metals is unknown. If necessary, we are forced to use the model local pseudopotential. The latter contains the fitting parameters - in our case, two. In order to find these parameters, some experimental point data is usually used to further calculate other characteristics with the help of the resulting model pseudopotentials. Experimentally measured characteristics we have only two: the coefficient of electrical resistance and the pressure, which is clearly not enough for the traditional implementation of the specified algorithm. Therefore, we did not use them in the future to select pseudopotential parameters. Instead, we chose the selection of pseudopotential parameters along the whole set of characteristics that were calculated in a wide range of temperatures and densities. This set was supplemented with the packing fraction parameters of Li and Be liquid metals at their melting temperatures. It should be noted that from these metals the second period of the periodic table, which includes both N and O, begins. Also we have considered the pair effective ion-ion interactions in the second and third order of perturbation theory. The criterion for the correctness of the dependencies of various characteristics of N and O on temperature and density was the similarity of this behavior to the behavior of the corresponding characteristics of liquid metallic hydrogen, as well as Li and Na. Such a requirement practically uniquely made it possible to select the values of two parameters of the model pseudopotential. The theoretical values of pressure and electrical resistivity, obtained by us for the declared by the authors of the discovery of metallic nitrogen and oxygen values of temperatures and densities, appeared to be quite satisfactory with the corresponding experimental data.

3-10.P

INFLUENCE OF NANOPARTICLES FIELDS AND EXTERNAL FIELDS ON CRITICAL PARAMETERS AND EQUATION OF STATE FOR CONDENSED SYSTEMS NEAR THEIR CRITICAL POINTS

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Earlier it was shown [1-3] that near the critical point ions can be surrounded by solvate shell, as a result of which part of the large-scale nanoscale fluctuations of the order parameter in the system becomes charged. Under this assumption, the interaction of ions with condensed system in the near-critical state can be represented as the interaction of "charged" nanosized fluctuations of the order parameter with "uncharged" ones.

It has been experimentally shown that temperature and concentration dependences of shear critical viscosity with the addition of ions [3] and Laponite nanoparticles to isobutyric acid-water solution within the experimental error quantitatively correspond to the equation of critical viscosity [4] with fixed value of the wave vector q=0,02 for all investigated concentrations of added charged particles. Wherein character of influence of ions and Laponite on critical parameters and equation of state of solution is similar and the condenced system is described by scaling equations of the state of the three-dimensional Ising model. From a microscopic point of view, Laponite is a mixture of nanodiscs, whose planes are charged negatively, and their edges are positive. It can be assumed that on the surface of the nanoparticles of the laponite there will be a distribution of charges of the opposite sign, which will result in the interaction of Laponite surrounded by the solvate shell with "uncharged" fluctuations of the solution. The weak interaction of the Laponite with the solution in comparison with the ion can be explained qualitatively by the model presentation that the Laponite discks enclosed by the solvate shell is due to the disk shape has a quadrupole moment; its interaction with the fluctuations of the solution isobutyric acid-water, which has a dipole moment, can be considered as quadrupole-dipole. At the same time, the interaction of the added positively or negatively charged ion, surrounded by a solvate shell with water and isobutyric acid, can be regarded as more intense coulomb-dipole. In both cases, it is assumed that the influence of the electric fields of particles added to the system is manifested on nanosized scale of charged fluctuations or nanodiscs surrounded by solvate shells. The proposed description corresponds to the conclusion of the fluctuation theory of phase transition [5] that the atomic and molecular degrees of freedom do not determine the behavior of the system in the near-critical state. It is experimentally shown that the addition of ions and Laponite to solution leads to a narrowing of the three-dimensional phase diagram of the correlation length both in temperature and concentration (or field), depending on the concentration of added to the system charged particles under the action of their electric field. Proceeding from the decisive role of the condenced system's correlation length, the phase diagrams of concentration, entropy, osmotic compressibility, heat capacity etc. are also deformed in accordance with the phase diagram of the correlation length.

The analysis has been shown that due to the increase of the critical temperature, this should lead to an increase in the magnitude of the effect of gravity [6]. The influence of electric fields of the ions or Laponite on liquid system results in more strong concentration dependence of the change in the electrochemical potential $\Delta\mu^*=(\mu-\mu_c)/(v_cP_c)$. The comparative analysis of the data on the effect of gravity and the data on the effect of ions and Laponite adding to the liquid system near the upper critical temperature leads to the conclusion that the effect of electric field intensity $E=-grad(\mu)=-grad(\mu^*)\cdot v_cP_c=-grad(P^*)\cdot P_c$ and gravity field intensity $g=-grad(\varphi_g)=-grad(h)\cdot M_r\cdot v_cP_c$ on the dimensionless gradient of electrochemical potential $d\mu^*/dh\sim E/g$ of the inhomogeneous system under gravity is diametrically opposite; it also should leading to width narrowing of the fluctuation region on variation of the hydrostatic pressure field parameter $h=\rho_c gz/P_c$. Further development of the proposed approach made it possible 1. to take into account the influence of charge and molecular weight of the moleculas; 2. to take into account the influence of constant magnetic field $H=-grad(\psi)$ with the help of the effective magnetic potential ψ in accordance with the approach [7], where the concept of the magnetogravitational potential is used; 3. to introduce the method for predicting the magnitude of the effect of gravity in the critical fluid for planets or in plasma with a non-Gaussian distribution function for stars.

References

[1] A.D. Alekhin, L.A. Bulavin, B.Zn. Abdikarimov, V.P. Kopylchuk, *Ukr. J. Phys.* **45(11)**, 1333 (2000).
[2] A.D. Alekhin, Ukr. J. Phys. **47(11)**, 1045 (2002).
[3] A.D. Alekhin, J.L. Ostapchuk, E.G. Rudnikov, A.V. Voyteshenko *Russian J. of Phys. Chem. A* **88(9)**, 1519 (2014).
[4] A.D. Alekhin , *Ukrainian Journal of Physics* **2**, 138 (2004).
[5] A.Z. Patashinskii, V.L. Pokrovskii Fluctuation Theory of Phase Transitions, Science, Moskow, 1982.
[6] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.
[7] R. Wunenburger, D. Chatain, Y. Garrabos, D. Beysens, *Phys. Rev. E* **62(1)**, 469 (2000)

3-11.P

DIFFUSION MODELS FOR IONIC LIQUIDS –ALCOHOL SOLUTIONS

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Extraction of alcohols from water solutions gains the increasing value thanks to a possibility of use of alcohols as additives to usual types of fuel. To meet safety requirements and not toxicity shown to extraction environments use in their quality of ionic liquids which have necessary. To answer a question of a possibility of use of ionic liquids as extracts it is necessary to analyze mechanisms of interaction of ionic liquid with alcohol. The MD was applied using a DL_POLY_4.05. The methyl-groups in the dmim+ were treated as a pseudo-atom with the total charge. All the studies were conducted for systems composed of 192 dmim+ cations, 192 chlorine anions Cl–, and one solute molecule at T = 400 K. The unit cell volume was calculated from the experimental values of the ionic liquid density at T = 400 K. The electrostatic interaction at short distances was described using point charges on each atom. The interaction between dmim+ and Cl– molecules in the ionic liquid was described using the Buckingham potential for interactions at short distances. The Berendsen thermostat was used to stabilize the system in the N V T -ensemble. Analysis of the data allowed to establish: (1) The salvation effect in systems ionic-liquid (dmim+/Cl-) - alcohols solute molecules (methanol, ethanol, propanol and butanol) have qualitatively similar to the behavior of water molecules in IL. (2) The results of the computer experiment for <Etot> for the dmim+/Cl– alcohols solutions at T = 400 K show that the intermolecular interaction <Etot> does depend on the physical characteristics of dissolved substances. In this case, need to do analysis also of its dynamic properties. (3) Based on the data obtained from MSD and VAF the different diffusion mechanisms of alcohol molecules in IL ware determined.

3-12.P

MOLECULAR RELAXATION IN BINARY SYSTEMS

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Investigation of the processes of molecular relaxation by the methods of vibrational spectroscopy provides the information on the structural and dynamical properties of condensed systems [1]. Such studies are based on the fact that the widths of bands in the vibrational spectrum are inversely proportional to the molecular relaxation times. The purpose of this study is to analyze and compare the processes of molecular relaxation in salt and binary systems, as well as to determine the possible additional mechanisms of relaxation of vibrationally excited states of molecular ions in binary systems. The objects of investigation were chosen as follows: salts $LiNO_3$, $LiClO_4$, $NaNO_3$, $NaClO_4$, KNO_3, $KClO_4$; systems $LiNO_3$–$LiClO_4$, $NaNO_3$–$NaClO_4$, KNO_3–$KClO_4$.

The processes of molecular relaxation in the binary nitrate–perchlorate systems have been investigated using Raman spectroscopy. It has been found that the relaxation time of the $\nu_1(A)$ vibration of the NO_3^- anion in the binary system is shorter than that in the nitrates. It has been shown that an increase in the relaxation rate is caused by the existence of an additional mechanism of relaxation of vibrationally excited states of the nitrate ion in the system. This mechanism is associated with the excitation of a vibration of another anion (ClO_4^-), as well as with the “creation” of a phonon. It has been established that the condition for the realization of the relaxation mechanism is that the difference between the frequencies of the aforementioned vibrations should correspond to the range of sufficiently high densities of states of the phonon spectrum.

References

[1] A.R.Aliev, I.R.Akhmedov, M.G.Kakagasanov, Z.A.Aliev, *J. Optical Technology*, **85**, 8-11 (2018).

3-13.P

THE EFFECT OF Mn ON THE VISCOSITY OF THE LIQUID Sn

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Due to unique physical and chemical characteristics tin could be placed among pure metals intensively applied in the production of industrial materials. For example, tin is the main component of lead-free solders insuring a good connection between assembly elements through chemical interaction between atoms of Sn and Cu resulted in formation of interfacial intermetallic compound layer between the solder and substrate. Minor addition of various impurities to pure tin is a very popular strategy to improve their microstructure and enhance properties. It could be either ceramic of metal additions [1,2].
The present study is aimed on investigation of the viscosity as a function on temperature and concentration. The measurements were performed by the oscillation crucible method. Based on temperature dependence of the viscosity the activation energy of viscous flow was estimated. The concentration dependence of the viscosity and activation energy of viscous flow was analyzed in respect to the phase diagram of the Mn-Sn system. Furthermore, experimental results were compared with calculated values using the Budai-Benko-Kaptay and the Schick et al. models. A good agreement between experimental and modeled data was obtained.
Financial support for this study came from the Austrian Science Fund (FWF) under project No. P27049-N19.

References

[1] A. Yakymovych, P. Svec Sr., L. Orovcik et al., *J. Electron. Mater.*, **45**, 6143-6149 (2016).
[2] A. Yakymovych, P. Svec Sr., L. Orovcik et al., *J. Electron. Mater.*, **47,** 117-123 (2018).

3-14.P

ATOMIC CHARGES FOR CONFORMATIONALLY RICH MOLECULES OBTAINED THROUGH A MODIFIED PRINCIPAL COMPONENT REGRESSION

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A modification of the principal component regression model is proposed for obtaining a fixed set of atomic charges (referred to as dipole-derived charges) optimized for reproducing the dipole moment of a conformationally rich molecule, i.e., a molecule with multiple local minima on the potential energy surface. The method requires geometry of the conformers, their dipole moments and APT charges (i.e., only the observable molecular properties) in each of the conformers as input data, and produces a single set of fixed charges suitable for accurate representation of both the dipole moment vector of all conformers and its variations resulting from small changes in molecular geometry (e.g., caused by vibrations) [1]. The peculiar feature of the method is that it requires neither adjustable empirical parameters, nor averaging over conformers or any other post-processing of the obtained charges. The input data used in the proposed method are obtained from *ab initio* calculations which also do not require empirical parameters.
The proposed method has been applied to canonical 2'-deoxyribonucleotides, the model DNA monomers, and the dipole-derived charges have been shown to outperform both the averaged APT and RESP charges in reproducing the dipole moments of large sets of conformers, thus demonstrating a potential usefulness of the dipole-derived charges as a 'reference point' for modeling polarization effects in conformationally rich molecules, parameterizing non-polarizable force fields and for developing novel polarizable force fields for classical MD simulations.
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References

[1] T.Yu.Nikolaienko and L.A.Bulavin, *Phys. Chem. Chem. Phys*, **20**, 2890–2903 (2018).

Section 4. Quantum Liquids

Oral session

4-1.O

BOSE-EINSTEIN CONDENSATION OF HETERONUCLEAR FERMI-FERMI MOLECULES IN A TWO-SPECIES FERMI GAS

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We theoretically study the phenomenon of Bose-Einstein condensation of heteronuclear Fermi-Fermi molecules formed in a two-species Fermi gas [1]. To this end, we employ a microscopic approach that involves the Bogoliubov model for a weakly interacting Bose gas and approximate formulation of the second quantization method in the presence of bound states of particles elaborated earlier by the authors [2]. The basic thermodynamic characteristics of the system such as the single-particle excitation spectrum, the ground-state energy, the densities of molecular condensate and unbound fermionic atoms are found. We specify the boundaries of the applicability of the developed microscopic approach. In order to bring the obtained results to real experimental conditions, we study a mixture of ^{6}Li and ^{173}Yb atoms, where the simultaneous quantum degeneracy was experimentally realized [3]. This mixture can be the basis for experimental creation of ultracold molecules.

References

[1] A.S. Peletminskii, S.V. Peletminskii, and Yu.V. Slyusarenko, *J .Phys. B: At .Mol. Opt. Phys.*, **50**, 145301 (2017).
[2] S.V. Peletminskii and Yu.V. Slyusarenko, *J. Math. Phys.*, **46**, 022301 (2005).
[3] H. Hara, Y. Takasu, Y. Yamaoka, J.M. Doyle, and Y. Takahashi, *Phys. Rev. Lett.* **106**, 205304 (2011).

TO TEMPERATURE DEPENDENCE OF HEAT CONDUCTIVITY AND VISCOSITY IN POLARON HYDRODYNAMICS

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Hydrodynamics of polaron subsystem of semiconductors is investigated on the basis of kinetic equation for polarons interacting with phonon subsystem. In is known that energy change of electrons in electron-phonon collision in the framework of the Fröhlich model is small (see, for example, [1]). Therefore, after free path time in electron and phonon subsystems states with some different temperatures are established. Then slow relaxation process of equalization of the polaron and phonon temperatures is observed. In this work phonon subsystem is assumed to be in an equilibrium with the temperature T_0 and dependence of polaron kinetic coefficients on polaron temperature is investigated.

Polaron distribution function $\mathrm{f}_p(x,t)$ is sought in normal form as a functional $\mathrm{f}_p(x,\xi(t))$ of polaron temperature $\xi_0(x,t)\equiv T(x,t)$, mass velocity $\xi_l(x,t)\equiv \upsilon_l(x,t)$ and density $\xi_4(x,t)\equiv n(x,t)$. As usual gradients of the hydrodynamic variables $\xi_\mu(x,t)$ are considered as small quantities (small parameter g). Distribution function $\mathrm{f}_p(x,\xi)$ in the leading in the first approximations in the gradients has the form

$$\mathrm{f}_p^{(0)} = w_p[1+g_p], \qquad w_p = \frac{n}{(2\pi m T_0)^{3/2}} e^{-\frac{\varepsilon_p}{T_0}}; \tag{1}$$

$$\mathrm{f}_p^{(1)} = w_p\left(C_{lp}E_l + D_{lp}\frac{\partial \ln n}{\partial x_l} + G_{lp}\frac{\partial T}{\partial x_l} + F_{slp}\frac{\partial \upsilon_s}{\partial x_l}\right) \tag{2}$$

with some functions of variables $\xi_\mu(x)$ which have to be found. Heat conductivity and viscosity of the polaron subsystem are given by formulas

$$\kappa_{nl} = -\frac{1}{m}\langle p_n \varepsilon_p G_{lp}\rangle, \qquad \eta_{nl,ms} = -\frac{1}{m}\langle p_n p_l F_{msp}\rangle \tag{3}$$

($\langle a_p\rangle$ denotes average of a quantity a_p with the distribution w_p). For the function g_p is obtained linear integral equation with additional conditions

$$a_l\frac{\partial g_p}{\partial \upsilon_l} + b\frac{\partial g_p}{\partial T} = \hat{K}g_p; \qquad \langle g_p\varepsilon_p\rangle = \frac{3}{2}n(T-T_0) + \frac{mn\upsilon^2}{2}, \quad \langle g_p p_l\rangle = mn\upsilon_l, \quad \langle g_p\rangle = 0 \tag{4}$$

($\hat{K}$ is operator of the collision integral, a_l, b are some coefficients that have to be found). In the present work solution of the problem (4) is found based on [2] for small $T-T_0$, υ_l i.e. at the end of the relaxation processes that introduces an additional small parameter μ in the theory. Coefficient functions in the distribution function (2) are found in a perturbation theory in this small parameter too that gives temperature dependence of the kinetic coefficients (3).

References

[1] A.I. Anselm, Introduction in Theory of Semiconductors, M.: Nauka, 1978, 615 p. (in Russian).
[2] S.A. Sokolovsky, On theory of nonlinear relaxation in polaron subsystem of polar semiconductors, In: Proceedings of the XXII[nd] International Seminar/Workshop on direct and inverse problems of electromagnetic and acoustic wave theory, 2017, P. 242-247.

4-3.O

EVOLUTION OF A TURBULENT PLUG IN A CHANNEL COUNTERFLOW OF SUPERFLUID 4HE

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I report recent results of a numerical study of the evolution of a localized quantum vortex tangle -a plug- in a channel counterflow of superfluid ^{4}He.
The unrestricted evolution of the turbulent plug in the channel was considered starting with its creation from few individual loops under counterflow conditions, followed by the decay at the same temperature until just few backbone vortices remained.
The simulations were performed using Vortex Filament method with full Biot-Savart description of the vortex line velocity at three temperatures and a number of counterflow velocities.
Unlike the unbounded homogeneous vortex tangles, the turbulent plugs in the channel remain anisotropic as they decay. Various statistical properties of the turbulent plug as well as the relative importance of different mechanisms affecting the local vortex line density are discussed.

4-4.O

NONADDITIVE GENERALIZATIONS OF QUANTUM ENSEMBLES

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Modifications of the conventional Bose-Einstein, Fermi-Dirac, and some intermediate types of statistics are presented [1-3]. Such generalizations are based on the nonadditive exponentials introduced in particular by Tsallis [4] and Kaniadakis [5]. Thermodynamic functions are calculated for some model systems with the specific heat serving as the best example to demonstrate peculiarities. The importance of fugacity definition is stressed for the discussed approaches being suitable for effective modeling of real physical systems.

References

[1] A. Rovenchak, *Phys. Rev. A* **89**, 052116 (2014).
[2] M. Ya. Hornetska and A. A. Rovenchak, *Ukr. J. Phys.* **61**, 168 (2016).
[3] Ya. Vasiuta and A. Rovenchak, *Physica A* **490**, 918 (2018).
[4] C. Tsallis, *Química Nova* **17**, 468 (1994).
[5] G. Kaniadakis, *Physica A* **296**, 405 (2001); *Entropy* **15**, 3983 (2013).

4-5.O

POSSIBILITY OF GENERATION OF A GIANT ELECTROMOTIVE FORCE BY THIRD SOUND

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It is predicted that oscillations of temperature during propagation of third sound in a thin superfluid film [1, 2] cause appearance of an alternating electric field in the surrounding space. The reason is that the non-stationary heating is accompanied by oscillations of film thickness. This causes oscillations of dipole moment of the film induced by the substrate and, as the result, appearance of oscillating electric field in the nearby space. The potential difference is proportional to the temperature gradient, i. e. a *non-stationary* thermoelectric effect must take place, that is impossible in normal systems. The magnitude of the effect depends significantly on the substrate type and coating and is practically insensitive to the vortex formation effects. The presence of thermally activated vortices leads only to renormalization of third sound speed [3] and their effect on the electric field caused by the third sound wave is weak even in the vicinity of the superfluid transition.

It is considered the region of low (TK 1) and high (TK 1) temperatures. For the low-temperature region, the electric field produced by the film is inversely proportional to the cube of the equilibrium film thickness h_0. For the high-temperature region, the generated electric field is independent of h_0. The last result is valid while the temperature addition T' creates a deviation h' satisfying the condition h' h_0.

It is shown that the differential thermal EMF (the ratio of electric potential amplitude to the film temperature amplitude), which is a characteristic of thermoelectric properties of a substance, can reach in the predicted effect 10^{-4} V/K. For pure non-magnetic metals this quantity has the order of 10^{-8} V/K (see e. g. [4]). Therefore the differential thermal EMF caused by third sound can be even called giant.

References

[1] K.R. Atkins, *Phys. Rev.* **113**, 962 (1959).
[2] I. Rudnick, R.S. Kagiwida and J.C. Fraser, *Phys. Rev. Lett.* **20**, 430 (1968).
[3] S. I. Shevchenko and A. M. Konstantinov, *JETP Lett.* **104**, 489 (2016).
[4] A.A. Abrikosov, *Fundamentals of the Theory of Metals*, North Holland, Amsterdam (1988).

4-6.O

ELECTRO-MECHANICAL PROPERTIES OF SUPERFLUID HELIUM

Valery Khodusov

In experiments [1], A.S. Rybalko discovered the electrical activity of superfluid helium. Rotons give the main contribution to the thermodynamic and kinetic values in the region where the experiments were carried out. The presence of bound electro-mechanical properties of He II can be explained by making the assumption of the presence of a dynamic dipole moment in the roton [2, 3].

In this paper, on the basis of this assumption, the total momentum and electric induction per a unit volume of helium were calculated with allowance for the additions to the energy of the roton that arise during the motion of a superfluid liquid and in the presence of an electric field. Knowing the thermodynamically equilibrium distribution function and using the standard methods of statistical physics, one can find all thermodynamic parameters and coefficients. Calculations show that the total momentum and electric induction linearly depend on the electric field E and the relative velocity of motion of the normal and superfluid components W. The free energy is found as a function of T, W, E.

References

[1] A. Rybalko, . S. Rubets, *Low Temp. Phys.* **31**, 623 (2005)
[2] Mineev, V.P. *Jetp Lett.* **90**, 768 (2010)
[3] Khodusov V.D., *Visn. Khark. Univ.*, 2004, 642, No. 3(25), 79

4-7.O

ABOUT CALCULATION OF SPECIFIC HEAT FOR DENSE SUPERFLUID NEUTRON MATTER WITH ANISOTROPIC SPIN-TRIPLET P-WAVE PAIRING AT LOW TEMPERATURES

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The analytical expression for specific heat of dense superfluid neutron matter (SNM) with anisotropic spin-triplet p-wave pairing is derived in the limit of zero magnetic field within the framework of generalized Fermi liquid approach (see, e.g., review [1], our article [2] and references therein). The obtained expression for specific heat $C_{SNM}(n,T)$ is valid for arbitrary parametrization of the effective Skyrme interaction in neutron matter and is nonlinear function of density n and temperature T (namely, $C_{SNM}(n,T) \sim T^3$) in limiting case of low temperatures $0 < T << T_{c0}(n)$ (where $T_{c0}(n)$ is phase transition temperature for dense neutron matter from normal to superfluid state). This function $C_{SNM}(n,T)$ is specified for generalized BSk21 [3] parametrization of the Skyrme forces (with additional terms dependent on density n) and figures are plotted at subnuclear and supranuclear densities on the interval $0.1 \cdot n_0 < n < 2 \cdot n_0$, where $n_0 = 0.17$ fm^{-3} is nuclear density.

References

[1] A.I. Akhiezer, V.V. Krasil'nikov, S.V. Peletminskii, and A.A. Yatsenko, *Phys. Rep.*, **245**, 1-110 (1994).
[2] A.N. Tarasov, *Fiz. Nizk. Temp.*, **42**, 222-229 (2016) [*Low Temp. Phys.*, **42**, 169-175 (2016)].
[3] S. Goriely, N. Chamel, and J.M. Pearson, *Phys. Rev. C*, **82**, 035804 (2010).

4-8.O

ONE-DIMENSIONAL SYSTEM OF POINT BOSONS: NEW SOLUTIONS

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We consider a one-dimensional (1D) system of N spinless point bosons in the exactly solvable approach, based on the Bethe ansatz. Using the Gaudin's numbering, we show that particle-like excitations are bosons. We calculate the partition function at $N=\infty$ for the periodic and zero boundary conditions and obtain the formula for the free energy of the system: $F = E_0 + T\sum_{I\neq 0}\ln(1-e^{-\frac{E_+(p_I)}{T}})$, where $E_+(p)$ is the dispersion law of particle-like excitations [1,2]. In this case, the solution for F takes into account all excited states of the system (i.e., both the particle-like and hole-like excitations). We compare our solutions with the solutions in the traditional Yang-Yang approach [3]. We note that the partition function of a 1D system of point bosons was not found previously.
We also obtain the formula for the quasimomentum of a quasiparticle under zero boundary conditions. Making use of this formula, we calculate the dispersion law of the particle-like and hole-like excitations under zero boundary conditions [4].

References

[1] M. Tomchenko, *J. Phys. A: Math. Theor.* **48**, 365003 (2015).
[2] M. Tomchenko, *J. Low Temp. Phys.* **187**, 251-266 (2017).
[3] C.N. Yang and C.P. Yang, *J. Math. Phys. (N.Y.)* **10**, 1115-1122 (1969).
[4] M. Tomchenko, *arXiv:*1705.10565 [cond-mat.quant-gas] (2017).

4-9.O

KORTEWEG FLUID AS EFFECTIVE DESCRIPTION OF CONDENSATE-LIKE SYSTEMS

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We apply statistical mechanics arguments and Madelung hydrodynamical presentation for an effective description of strongly-interacting many-body systems [1-3]. A Schrodinger-like wave equation with logarithmic nonlinearity is shown to appear in such systems [4]. It describes the irrotational and isothermal flow of a two-phase barotropic compressible inviscid Korteweg fluid with internal capillarity [5]. We demonstrate spontaneous symmetry breaking in this class of fluids, which leads to fluid fragmentation and nucleation of density inhomogeneities. We show that density inhomogeneities occur which are described by solitary wave solutions with a Gaussian density profile. We derive the many-body interaction potential for collective degrees of freedom corresponding to theses inhomogeneities.

References

[1] A. V. Avdeenkov and K. G. Zloshchastiev, *J. Phys. B: At. Mol. Opt. Phys*. **44**, 195303 (2011).
[2] K. G. Zloshchastiev, *Acta Phys. Polon*. B **42**, 261 (2011).
[3] Yu. A. Rylov, *J. Math. Phys.* **40**, 256 (1999).
[4] S. De Martino, M. Falanga, C. Godano and G. Lauro, *Europhys. Lett*. **63**, 472 (2003).
[5] J. E. Dunn and J. Serrin, *Arch. Rat. Mech. Anal*. **88**, 95-133 (1985).

Poster session

4-1.P

QUADRATIC APPROXIMATION IN THEORY OF A WEAKLY INTERACTING BOSE GAS WITH CONDENSATE: THE ROLE OF NON-LOCAL INTERACTION POTENTIALS

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We derive and analyze the general coupled equations of quadratic approximation of the Bogoliubov model for a weakly interacting Bose gas. The first equation determines the condensate density as a variational parameter and ensures the minimum of the grand thermodynamic potential. The second one represents the equation for the total number of particles. Their consistent analysis is performed for a number of model interaction potentials including contact (local) interaction as well as potentials with finite range of interaction and nontrivial dependence of their Fourier transforms on momentum. As the latter case, the Gaussian and semi-transparent spheres potentials are considered. We demonstrate that the general equations of quadratic approximation have no solutions for a local potential, although they formally reproduce the well-known results such as the gapless spectrum of single-particle excitations as well as corrections to the condensate density and chemical potential in terms of the gas parameter. At the same time, it is shown that these equations have stable solutions if we consider more "realistic" non-local potentials. We show that in the regimes close to experimental realizations with ultracold atoms, the contribution of the terms originating from the quadratic part of the truncated Hamiltonian to the chemical potential can be of the same order of magnitude as from its c-number part. Due to this fact, in particular, the spectrum of single-particle particle excitations exhibits a gap.

4-2.P

NONLINEAR BEHAVIOR OF THE OSCILLATING TUNUNG FORK IN HE II UNDER QANTUM VORTICES – PHONON SCATTERING

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Experiments have been carried out on the excitation of hydrodynamic flows in superfluid helium under forced vibrations of a quartz tuning fork immersed in a liquid. Nonlinear oscillations that arise with an increase in the driving force are investigated and are manifested by distortion of the shape of the resonant amplitude-frequency characteristic in comparison with Lorentz curves typical for an extremely small force. Nonlinear resonance curves are described using the Duffing equation [1], the parameters of which are established by comparing the theoretical calculation with the experimental data.

Dependence of the velocity of vibrations of the tuning fork legs on the driving force established with the use of the Duffing equation, is close to the dependence previously obtained for the quasi-laminar flow of He II and containing a cubic velocity contribution due to the mutual friction caused by scattering of phonons by quantized vortices in a turbulent flow.

References

[1] L.D Landau, E.M Lifshits, "Mechanics", Moscow, Nauka (1988).

4-3.P

DRAG COEFFICIENT OF QUARTZ TUNING FORK IN SUPERFLUID ^{3}He - ^{4}He MIXTURES

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The impurity ^{3}He particles are actually the only factor influencing the properties of ^{4}He. The purpose of this study is the investigation of the effect of impurity particles on the damping of a quartz tuning fork, oscillating in the laminar flow of concentrated superfluid, ^{3}He-^{4}He mixtures and to determine the main mechanisms of kinetic energy dissipation the region of high ^{3}He concentrations. The temperature dependences (from 0.5 to 2.5 K) of resonance curves of a quartz tuning fork with resonant frequency of 32 kHz in solutions of helium with concentrations of ^{3}He of 1%, 5% and 15% in the laminar flow region.

The results obtained were used to plot the temperature dependence of the drag coefficient. With the help of the normalization on the effective area of the oscillating body, the concentration dependence of the drag coefficient of the quartz tuning fork and the vibrating sphere [1] in superfluid solutions has been constructed and analyzed.

Comparison of drag coefficients with the calculated contributions of viscosity and the first sound attenuation indicates the presence of excessive dissipation in the experimental values. It was found that the viscous contribution exceeds the contribution of the first sound only at T > 1.5K. These contributions are approximately equal below 1.5K. The presence of excess attenuation indicates the presence of additional dissipation mechanisms. The first candidate is the radiation of the second sound which also exists in ^{3}He–^{4}He solutions. Its role increases with increasing the concentration of ^{3}He [2], but this contribution does not have an analytical expression yet.

References

[1] H. Kerscher, M. Niemetz, W. Schoepe, J. Low Temp. Phys. **124**, 163-168 (2001).

[2] V.A. Bakhvalova, I.A. Gritsenko, E.Y. Rudavskii, V.K. Chagovets, G.A. Sheshin, Low Temp. Phys. **41**, 502-509 (2015).

4-4.P

OF COLLECTIVE PROPERTIES OF VALENT OSCILLATIONSC-H AND O-H BONDS IN SOLUTIONS CH_3OH WITH $CHCl_3$

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The report analyzes the features of the formation of high-frequency (HF) vibrational bands (VB) of valent vibrations of the lengths of C-H and O-H bonds both in pure liquids $CHCl_3$ and CH_3OH, and in their solutions. This problem has to do with the problem of the formation and spectral manifestations of hydrogen bonds (HB) in liquids. The IR absorption and Raman scattering (RS) (710 nm) spectra of solutions of $CHCl_3$ with CH_3OH at different concentrations of C were studied. The characteristic VB in the region of the ν_{CH} and ν_{OH} oscillations are illustrated in Figs. 1a and 1c. The OH group in the CH_3OH molecule lowers the symmetry of the methyl group from C_{3V} to C_S. Therefore, the vibration of $\nu_{CH}(E)$ splits into oscillations of types A' and A", which is confirmed by the results of quantum chemical calculations with allowance for anharmonicity (B3LYPultrafine/cc-pVTZ). The frequencies of the three vibrations of the CH_3 groups obtained are shown by the arrows in Fig. 1a. It also shows the structure of VB in the region of $\nu_{CH}(E)$ CH_3OH and $\nu_{CH}(\nu_1)$ $CHCl_3$ and the additional band ~ 3075 cm^{-1} $CHCl_3$ (insert). The resulted interpretation of the lines $\nu_{CH}(A')$=2943-2948 cm^{-1} and $\nu_{CH}(A")$=2989-2991 cm^{-1} [1] looks doubtful, since these frequencies exceed the calculated values for single molecules of 2932 and 2965 cm^{-1}.

Using the results of a numerical expansion of the VB set into Lorentzians, the concentration dependences of the frequencies ν, the half-width $\delta\nu$, and the intensities of all the structural components have been studied, which is partially shown in Figs. 1b and 1c. Figure 1b shows the dependences of $\delta\nu(C)$ for all C-H bond vibrations in CH_3OH and $CHCl_3$ molecules. We point out that the half-widths of the three main components are much smaller than $\delta\nu$~40-60 cm^{-1} for the additional components $\nu_{1,2,3}$. A characteristic feature of the components $\nu_{1,2,3}$ is the attainment of maxima $\delta\nu$ at C≈40-60vol%. The additional components ν_{OH}'=3637-3645 cm^{-1}, $\nu_{OH}"$=3630-3635 cm^{-1} are found in the HF region of the broad band of 3200-3600 cm^{-1} O-H bonds (see Fig. 1c). On the special origin of the components $\nu_{1,2,3}$ and ν_{OH}', $\nu_{OH}"$, in addition to the maxima $\delta\nu$, the maxima of the frequencies and intensities also indicate that it is partially shown in the insets in Fig. 1c.

It is important that the frequencies ν_{OH}' decrease with increasing $C(CH_3OH)$ and they can not be referred to oscillations of free O-H bonds. We connect additional HF components near the main lines $\nu_{CH}(A_1)$, $\nu_{CH}(E)$ ν_{CH} and ν_{OH} with the existence of quasiphonon branches $\nu(\mathbf{k})$ with positive dispersion ($d\nu/d\mathbf{k}$>0). The widths of the corresponding phonon bands in the order of increasing frequency are ~80, 110, 150 and 260 $см^{-1}$.

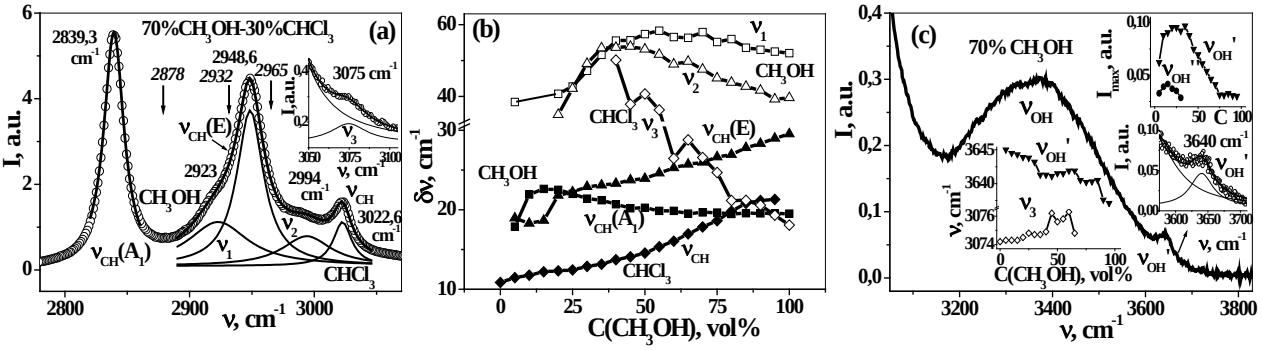

Fig.1. The structure of VB of C-H oscillations at C (CH_3OH) = 30vol% (a), the $\delta\nu$ (C) dependence for all ν_{CH} (b) components and the ν_{OH} band with the HF component ν_{OH}' with the dependences ν(C) and I_{max}(C) (insert) (c).

References

[1] L.M. Sverdlov, M. A. Kovner, E. P. Krainov, Vibrational Spectra of Polyatomic Molecules, Wiley,New York, 1974

4-5.P

ELECTRIC CURRENT IN THE WIGNER CRYSTAL IN A NARROW CHANNEL

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Modeling of electric current in the spatially ordered system of surface electrons over liquid helium (Wigner crystal) in a narrow channel are performed by the molecular dynamics method [1]. It is shown that electric field, applied to the electron system under measurements can result in the essential spatial rearrangement of the electrons. The rearrangement yields the measured electric current. It is shown that under certain conditions the electrons can leave the channel overcoming an energy barrier. That leads to the current spikes. As a result of comparison our results with the published experimental data we conclude that observed phenomena are due to electron-electron interaction and external electric fields, mainly and do not rely to features of the electron-ripplon interaction.

References

[1] V. Syvokon, I. Sharapova, *Fiz. Nizk. Temp*., **43**, 1303-1315 (2017).

THEORY OF THE PHOTOACOUSTIC EFFECT WITH SUPERFLUID SOLUTION ^{3}HE-^{4}HE

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The one-dimensional theory of the generation of a photoacoustic (PA) signal by isotropic solids and classical liquids [1], when the detection of the signal is carried out by a gas-microphone method, has shown the wide possibilities of this method for measuring the kinetic, acoustic and thermodynamic parameters of various systems, which has been repeatedly confirmed experimentally (see, for example, [2,3]). However, direct application of the results of this theory to describe the features of the generation of a PA signal in the superfluid He^3-He^4 solution is not possible. This is due to the following three circumstances: first, in superfluid liquids the heat conduction equation is hyperbolic, while in solids and classical liquids the parabolic equation; second, at the boundary of the solid body-the superfluid He^3-He^4 solution-there is a temperature jump discovered by Kapitza; third, the heat flux in the superfluid solution contains a convective component [4]. The purpose of this paper is to develop the theory of generating a PA signal by a superfluid solution into a buffer gas, when the detection of the signal is performed by a microphone method.

Suppose that the PA cell is filled with a superfluid He^3-He^4 solution, which is in equilibrium with its own vapor or pairs of one of the isotopes. The laser beam modulated in harmonic fashion with frequency ω and intensity I_0 perpendicularly falls on the PA cell. We consider the gas and the substrate to be transparent. We proceeded from the system of the heat equation for the gas layer, sample, and substrate. The solution of the boundary problem made it possible to find the temperature oscillation in the gas layer, by averaging which we found the following expression for the pressure oscillations in this layer

$$\delta p(\omega)=\frac{Y\alpha(1+i)\mu_g}{\alpha^2+\tilde{q}_2^2}\left[\frac{(s+b)(i\tilde{q}_2-\alpha)e^{i\tilde{q}_2 l}-(s-b)(i\tilde{q}_2+\alpha)e^{-i\tilde{q}_2 l}+2(\alpha s-ib\tilde{q}_2)e^{-\alpha l}}{(g+1)(s-b)e^{-iq_2 l}+(g-1)(s+b)e^{i\tilde{q}_2 l}}\right.$$

Here $Y=\gamma p_0 I_0(\tilde{\sigma}-\beta\alpha_T u_1^2)/[4T_0 l_g\rho_0\sigma_0 C_p\tilde{u}_2]$, γ - ratio of specific heat, p_0 - ambient pressure of gas, $s=1-k_b\sigma_b R_k$, $\tilde{q}_2=\omega/\tilde{u}_2,\sigma_j=(1+i)\mu_j^{-1}$; $\tilde{u}_2=u_2\sqrt{1-\varepsilon}$, $\varepsilon=\beta\alpha_T u_1^2/\bar{\sigma}$; κ_i, C_{Pi}. $\mu_j(\omega)=\sqrt{(2\chi_j/\omega)}$ and $\chi_j=(\kappa_j/\rho_j C_{pj})$ - coefficients of thermal conductivity, specific heat, length of thermal diffusion and coefficient of thermal diffusivity of the corresponding layers; $\rho_0=\rho_s+\rho_{n.}$, ρ_n,ρ_s- the density of the superfluid and normal components, respectively; $u_{1,2}$ - the speed of the first and second sounds, respectively: α_T - is the coefficient of thermal expansion, σ_0 and c_0 - is the equilibrium value of the specific entropy and concentration; $f=0.5\alpha I_0 e^{i\omega t}e^{\alpha z}$, $\alpha=\alpha_1(1-c_0)+\alpha_2 c_0$, $\alpha_{1,2}$ are the optical partial absorption coefficients of the components He^4 and He^3, respectively; R_k - is the Kapiza resistance value for a given solution;

$$g=\frac{ik_g\sigma_g}{k\tilde{q}_2},\ b=\frac{k_b\sigma_b}{ik\tilde{q}_2[1+\varepsilon_1]},\varepsilon_1=\frac{i\rho\ C_p\tilde{u}_2^2}{\omega\kappa T_0\tilde{\sigma}}[T_0\sigma_0+c_0(\frac{Z}{\rho_0}+B)],\cdot\beta=\frac{\bar{\sigma}}{\rho_0}(\frac{\partial\rho}{\partial T})_{Pc}(\frac{\partial T}{\partial\sigma})_{Pc}+\frac{c_0}{\rho_0}(\frac{\partial\rho}{\partial c})_{PT};$$

l_b, l and l_g - are the thickness of the substrate, sample and gas layer, respectively.

The analysis of the obtained expression is performed and the features of the frequency dependence of the amplitude and phase of the generated PA - signal are established.

References

[1]. A. Rosencwaig A., Gersho A., *J. Appl. Phys.*, **47,** 64-69 (1976).
[2]. Gusev V.E., Karabutov A.A. Laser optoacoustic. New York:, AIP. 1993.
[3]. Egerev S.E., Lyamshev L.M., Puchenkov O.V., *Physics Uspekhi*, **33**, 739-762 (1990).
[4] Esel'son B N., Grigor'ev V.G., Ivantsov B.N and at. Solutions of quantum liquids He^3-He^4 (in Russian) M. Nauka, 424p, 1973.

4-7.P

CRITICAL VELOCITY OF TRANSITION TO TURBULENT STATE IN SUPERFLUID SOLUTIONS OF ^{3}He - ^{4}He

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The critical velocity of the transition from laminar to turbulent flow in superfluid ^{3}He solutions in ^{4}He has been determined in the temperature range 0.5-2.5 K at the saturated vapor pressure. To determine the critical velocity, the method of an oscillating quartz tuning fork immersed in a liquid was used. The amplitude-frequency and current-voltage characteristics of quartz tuning forks with a resonance frequency of 32 kHz in solutions of helium isotopes with a concentration of 1% and 15% ^{3}He in the normal and superfluid state were measured. To detect the transition to a turbulent state, measurements were performed in a wide range of excitation voltages, $5 \cdot 10^{-2}$ - 300 Vpp, which corresponds to an exciting force of 10^{-7} - 10^{-3} N.

The transition from laminar to turbulent flow at constant temperature was determined from the kink in the dependence of the resonance frequency and the maximum resonance amplitude, as well as the width of the resonance at half the maximum amplitude from the exciting force.

The obtained data were used to construct the temperature dependence of the critical velocity of the transition to the turbulent state of the normal and superfluid solution of ^{3}He in ^{4}He. An analysis of the results obtained showed that the addition of impurity particles ^{3}He increases the stability of liquid helium to form a turbulent state.

SPECTRAL DETECTION OF PHONON DISPERSION OF VIBRATIONAL MODES IN SOLUTIONS $CHCl_3$ WITH CH_3OH

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The detection of longitudinal-transverse (LO-TO) splitting for the ν_5(E) mode of liquid chloroform ($CHCl_3$) in vibrational spectra [1] raises the problem of phonon bands (PB) detection in liquids and quasivents of the phonon dispersion $\nu(\mathbf{k})$, where **k** - wave vector. The solution of this fundamental problem is based on a careful analysis of the forms of a number of vibrational bands (VB) of liquid $CHCl_3$ and its solutions with CH_3OH in the IR absorption and Raman scattering (RS) spectra. Figure 1a shows doublet VB $2\nu_4$ (2405 and 2437 cm^{-1}) in RS (insert) and $\nu_1+2\nu_4$ (5374 and 5414 cm^{-1}) in IR spectra. The similarity of these bands, as well as $\nu_1+\nu_4$ (4214 and 4255 cm^{-1}), indicates the general nature of their high-frequency (HF) spectral components (SC). We explain this by the existence of quasiphonon branches $\nu(\mathbf{k})$ with positive dispersion ($d\nu_4/d\mathbf{k}>0$) and the resolution of vibrational states (VS) near the edge of the Brillouin zone (BZ) in bands of the second and higher orders. In this case, the shifts of the HF satellites ~20-50 cm^{-1} are related to the widths of the phonon bands of liquid $CHCl_3$. This is confirmed by the discovery of similar HF components 1236-1237 cm^{-1} for solutions with methanol in the region of a sharp single band ν_4=1216 cm^{-1} in pure $CHCl_3$, which is shown in Fig. 1b. Observation of $\nu_4(\mathbf{k})$ in the region of the main bands of $CHCl_3$ is due to the distortion of the structure of the liquid in solutions.

The shape of the bands $CHCl_3$ ν_4(E), $\nu_2(A_1)$, their overtones $2\nu_4$, $3\nu_4$, and $2\nu_2$, as well as the total tones $\nu_1+\nu_4$, $\nu_1+2\nu_4$ in IR and RS spectra, is studied in detail with the numerical decomposition on the SC. Concentration dependences of the frequencies ν, the half-width $\delta\nu$, and the intensities of individual SC, as well as the general spectral splittings $\Delta\nu$ of all the analyzed bands, which determine the widths of the PB, are obtained. The obtained results are partially shown in Fig. 1c: for the phonon band $\nu_4(\mathbf{k})$, the width $\Delta\nu_4$=18-25 cm^{-1}, and for $\nu_2(\mathbf{k})$ $\Delta\nu_2$~10 cm^{-1}. The dependence of $\Delta_{LT}(C)$ LO-TO splitting for the ν_5 $CHCl_3$ mode is also shown here. A significant increase in $\Delta\nu_4$ and intermolecular interactions in the region of higher VS is established. The work opens a new direction in the study of the liquid state of matter and opens the way to the unification of fiqhic, chemistry, biology and medicine.

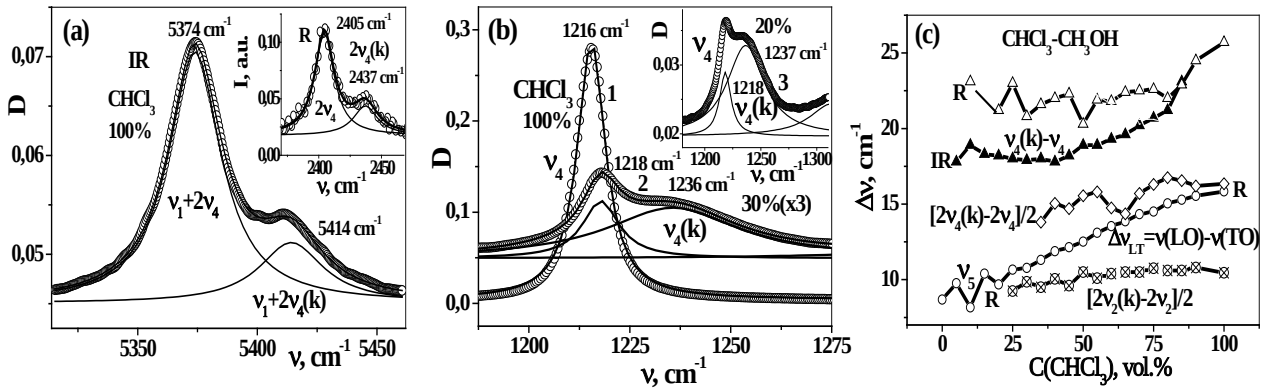

Fig.1. VB $2\nu_4$ in RS (insertion) and $\nu_1+2\nu_4$ in IR absorption (a), ν_4 of liquid $CHCl_3$ (1) and solutions with CH_3OH at a concentration of 30% (2) and 20% (insertion) in RS (b), and also concentration the dependence of the widths of the PZ mode ν4, determined from the bands ν_4, $2\nu_4$, $\nu_1+\nu_4$, $\nu_1+2\nu_4$ (c). Figure 1c. also shows the values of Δ_{LT} for the mode ν_5 and the width of the PZ for the ν_2 $CHCl_3$ mode.

References

[1] N.E.Kornienko, *Ukr. J. Phys.*, **46(5-6)**, 546-552 (2001).

Section 5. Binary Solutions. Polymer and Biopolymer Solutions

Oral session

5-1.O

HYDRATION OF DNA COUNTERIONS: A MOLECULAR DYNAMICS STUDY

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The structure of DNA double helix is known to be stabilized by water molecules and positively charged counterions. The interplay between water molecules and counterions in the ion-hydrate shell is the determinative feature for the understanding of many physical mechanisms of DNA biological functioning [1]. In the present work the molecular dynamics simulations have been carried out to study the impact of water molecules on counterions distribution around the double helix. The simulated systems consisted of DNA fragment d(CGCGAATTCGCG) in water solution with the counterions Na^+, K^+, Cs^+ or Mg^{2+}. The characteristic binding sites of the counterions with DNA and the changes in their hydration shell have been determined. The results show that due to the interaction with DNA at list two hydration shells of the counterions undergo changes. The first hydration shell of Na^+, K^+, Cs^+, and Mg^{2+} counterions in the bulk consists of 6, 7, 10, and 6 water molecules, respectively, while the second one has several times higher values. The Mg^{2+} and Na^+ counterions, constraining water molecules of the first hydration shell, form with DNA water-mediated contacts mostly. In this case the coordination numbers of the first hydration shell do not change while the coordination numbers of the second one decrease about twice. The Cs^+ and K^+ counterions that do not constrain surrounding water molecules may be easily dehydrated, and interacting with DNA their first hydration shell may be decreased by 3 and 5 water molecules, respectively. Due to the dehydration effect these counterions can squeeze through the hydration shell of DNA to the bottom of the double helix grooves and be there up to 10 ns. In this timescale the counterions may be accumulated in the minor groove forming a regular structure along DNA. The obtained results agree with the previous simulations and modeling data [1-3].

References

[1] M. Pasi, J.H. Maddocks, R. Lavery, *Nucleic Acids Res,*. **43**, 2412-2423 (2015).
[2] S.M. Perepelytsya, S.N. Volkov, *J. Mol. Liq.*, **164**, 113-119 (2011).
[3] O.O. Liubysh, A.O. Vlasiuk, S.M. Perepelytsya, *Ukrainian Journal of Physics*, **60** 433-442 (2015).

5-2.O

MODEL BIO-MEMBRANES STUDIED BY NEUTRON DIFFRACTION

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Small-Angle Neutron Diffraction (SAND) has over the recent years proven to be a useful technique in structural biology, biophysics and materials science. Due to the intrinsic disorder present in biomimetic samples - a disorder possibly important for the proper function of biology systems - many membrane samples are far from being perfect crystals. In such cases, less than atomic resolution structures are best described by broad statistical distributions, rather than sharp delta functions typical of perfect crystals. This is especially true for the structure of non-crystalline biomaterials with a focus on the most important "soft" matter studied, namely the lipid membrane.
Our recent experimental data revealed several intriguing peculiarities in structural properties of biomimetic membranes that will be discussed. Interestingly, one of the common alteration that is observed at the membrane-water interface underlines the important role of membrane hydration properties. A plausible mechanism of action in the case of many membrane additives seems to be in shifting the water encroachment the way that bilayers absorb more or less water molecules - one of the smallest and often neglected biomolecule. Although a complete understanding of the physicochemical processes taking place in biomembranes has yet to be established, an understanding of lipid bilayer structural changes as a result of different properties of environment outside and/or inside the membrane provides a foundation for better insights into the structure-function relationships that most certainly take place in more complicated biomembrane systems.

5-3.O

EFFECTIVE ELECTRICAL CONDUCTIVITY OF COMPOSITE POLYMER ELECTROLYTES

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It has been shown numerically [1] that the effective electrical conductivity of composite polymer electrolytes can be adequately described by considering such systems as dispersions of hard-core–penetrable-shell particles. The shells are introduced to account for the formation of highly conductive amorphous (with a decreased degree of crystallinity) regions around the filler particles. We use the compact-group approach [2,3] to give a self-consistent analytical solution to this model in the case where (a) the shells are inhomogeneous and characterized by an isotropic conductivity profile, and (b) the local value of the conductivity in the system is determined by the shortest distance from the point of interest to the nearest particle. The effective conductivity is expressed in terms of the constituents' conductivities and volume concentrations; the latter are determined by the statistical microstructure of the system. Our theory effectively incorporates many-particle effects and is expected to be rigorous in the quasistatic limit. Using the well-tested statistical physics results for the shell volume concentration, we support this conclusion by mapping our solution on 3D random resistor network simulations [1]. Finally, we apply our theory to a number of real PEO- and OMPEO-based polymer electrolytes to describe the nontrivial behavior of their effective conductivities as functions of the filler concentration and temperature.

References

[1]W. Wieczorek, M. Siekierski, Composite Polymeric Electrolytes, in Nanocomposites. Ionic Conducting Materials and Structural Spectroscopies, edited by P. Knauth and J. Schoonman (Springer, New York, 2008), pp. 1–70.
[2]M. Ya. Sushko, *Zh. Eksp. Teor. Fiz.*, **132**, 478 (2007). [JETP, **105**, 426 (2007)].
[3]M. Ya. Sushko, *Phys. Rev. E*, **96**, 062121 (2017).

5-4.O

MODELING OF STRUCTURAL RELAXATION IN THE GLASS TRANSITION OF POLYMER NANOCOMPOSITES FILLED WITH CARBON NANOTUBES

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The influence of carbon nanotubes (CNT) on enthalpy relaxation kinetics of polymethylmetacrylate (PMMA) is studied by the method of differential scanning calorimetry. The improved phenomenologic model for description of the structural relaxation of amorphous polymers in the glassing area is offered. The kinetic parameters of enthalpy relaxation for neat PMMA and nanocomposites which contained from 0,2 to 2 % carbon nanotubes were got from calculations. The fact of the infinite cluster formation were set from the changes of kinetic relaxation parameters. The features of polymeric composites' structure influence on their thermophysical properties are studied.
From the results it follows, that the process of enthalpy relaxation in the glazing of the PMMA/CNT system in general can be described with sufficient accuracy in the framework of Moinhen's model.
It was found that the most energy-stable structure is obtained when filling 0.5%. This is due to the formation of a leading cluster of particles of CNT.

5-5.O

EFFECT OF CHLOROPHYLLIN ON INTERACTION OF DYES WITH DNA

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Chlorophyllin (Chln) is able to reduce the mutagenic activity of DNA-binding dyes. The main molecular mechanism of its action is heteroassociation with toxic ligands (interceptor mechanism) [1]. The effectiveness of the Chln action depends on the dye-Chln and dye-DNA binding parameters ratio.
In this work, we studied the heteroassociation of berberine (Be), doxorubicin (Dox), methylene blue (Mb) and proflavine (Pf) with Chln and their interaction with DNA by spectrophotometric titration. The spectra of free Chln and dyes as well as complexes of dyes with an interceptor and DNA usually overlap; therefore, to analyze the obtained experimental data the principal component analysis SVD-ALS was used [2]. This allowed us to determine the concentrations of absorbing particles in the solutions and calculate the constants of dye-Chln heteroassociation and dye-DNA binding in the ternary dye-Chln-DNA systems and binary dye-Chln and dye-DNA systems.
The binding constants of the studied dyes with DNA are comparable with their heteroassociation constants with Chln. The effective binding constants of the dyes with DNA in ternary systems with Chln are smaller than the corresponding constants obtained for dye-DNA systems. The results of the study indicate that Chln is a good interceptor of the investigated dyes and can be used to reduce their toxicity.

References

[1] R. J. Epstein, *J. Clin. Oncol.* **8**, 2062-2084 (1990).
[2] K. H. Esbensen, D. Guyot, F. Westad, and L. P. Houmoller, *CAMO Process AS* (2002).

5-1.P

THERMALLY INDUCED GELATION IN AQUEOUS SOLUTIONS OF HYDROXYPROPYLMETHYLCELLULOSE

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We investigated the viscosity, heat capacity, and turbidity of aqueous solutions of hydroxypropylmethylcellulose (HPMC, Metolose SH65-50). The flow curves were obtained on the VSN-3 viscometer for HPMC mass concentrations of 2%, 2.5%, 3%, and 3.2% in the temperature range of 20-80°C and rotor speed of 200, 300, 400, and 600 rpm. The figure 1 shows the results of our experiments.

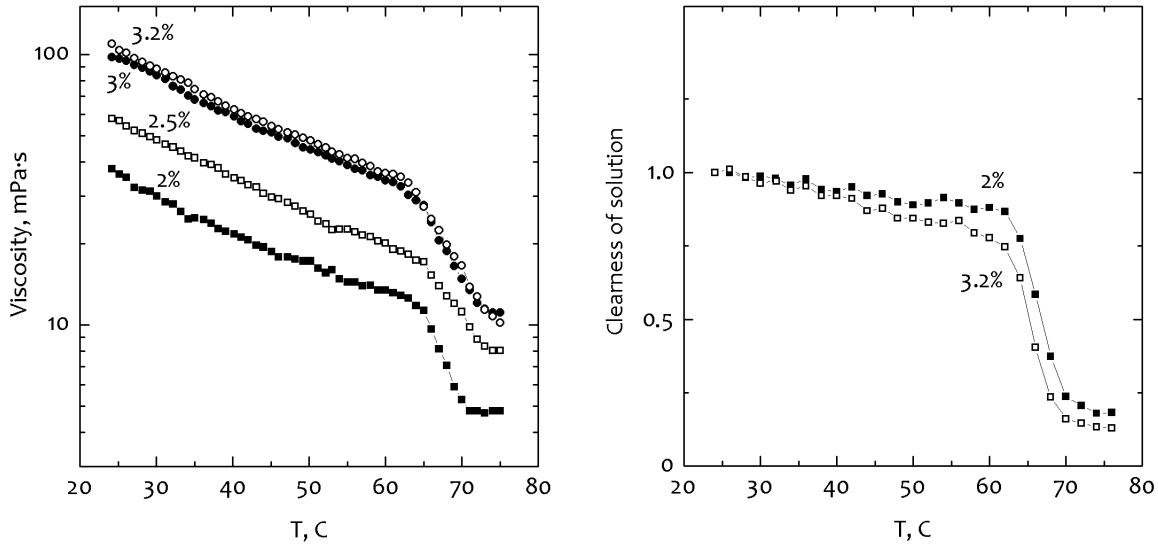

Fig. 1. Temperature dependences of viscosity (left) and turbidity (right) of HPMC aqueous solutions.

In our opinion, the observed structural transition is associated with a change in the fractal dimension of the grid of hydrogen bonds in H_2O with increasing temperature [1,2 and the Refs. therein]. This change leads to a violation of the balance between the intramolecular hydrogen bonds and the H-bonds of the molecule and the solvent.

References

[1] F. Tanaka and M. Ishida, *J. Chem. Soc. Faraday Trans.*, **91(16)**, 2663-2670 (1995).
[2] J. Patrick A. Fairclough et al., *Langmuir*, **28**, 10551-10557 (2012).

5-2.P

ELECTRICAL AND OPTICAL PROPORTIES OF POLYETHYLENE COMPOSITES WITH MULTI-WALL CARBON NANOTUBES

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Polymers, due to satisfactory mechanical properties, high plasticity, relatively low cost, are used in many technological processes. However, the vast majority of them have low electrical and thermal conductivity and are diamagnetic. To improve these and other characteristics, the introduction into the polymer matrix of multi-wall carbon nanotubes.

The aim of the work is to improve the conductivity, of polyethylene composites with 0-15 wt. % multi-wall carbon nanotubes; research of their structure; Raman Spectra and photoluminescence; the dependence of specific conductivity in the composite on temperature and frequency in the temperature range from -150 ℃ to + 125 ℃ by the method of an AC bridge at fixed frequencies: 5 GHz, 10 GHz, 20 GHz, 50 GHz. In the future it is planned to study the influence of the methods of making samples and changes of physical and chemical properties after irradiation. The results obtained will be useful for comparing and analyzing the influence of manufacturing and subsequent modification of samples.

STIMULI-RESPONSIVE ADSORPTION OF POLY-(2-DIMETHYLAMINOETHYL METHACRYLATE) ONTO SILVER NANOPARTICLES: MOLECULAR DYNAMICS SIMULATION STUDY

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Stimuli-responsive polymers contain ionizable groups that can dissociate into polyvalent macroions and counterions of opposite charges. Electrostatic interactions between charges lead to complex intra- and intermolecular interactions that have strong consequences for both static and dynamic properties of polyelectrolyte solutions, which are qualitatively different from those of conventional neutral polymers [1]. These features open up some advanced applications of stimuli-responsive polymers for the chemical modification of silver nanoparticles (AgNPs) by adding a novel functionality to smart sensing and delivery systems.

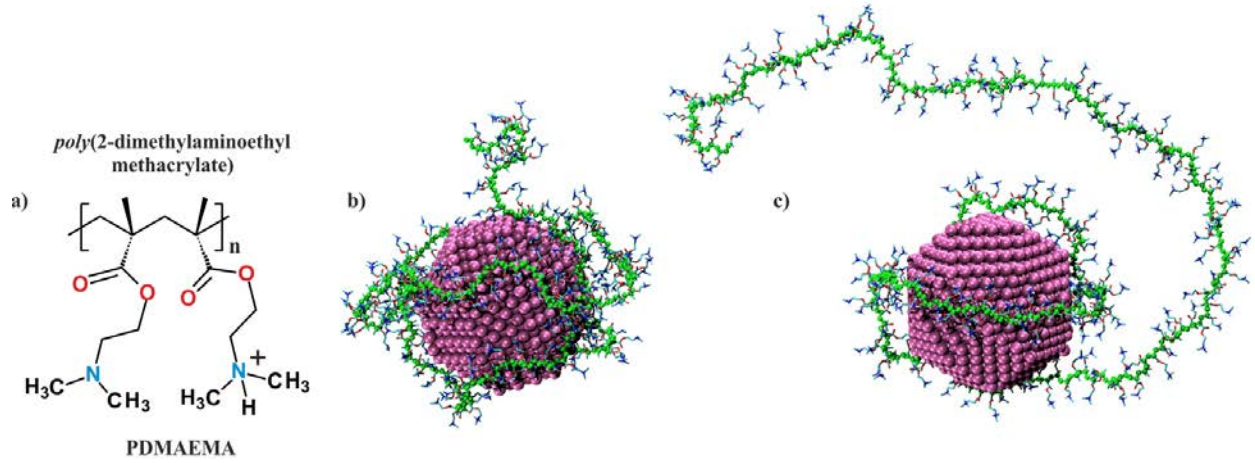

Figure 1. Molecular structure of PDMAEMA (*a*). MD snapshots of $AgNP_{1397}$ coated by $PDMAEMA_{220}$ with α=0 (*b*) and α=1.0 (*c*)

In this study, the adsorption behavior of a pH-responsive polymer PDMAEMA (Fig. 1) onto AgNP was studied as a function of a chain length (*n*=220-440) and a degree of protonation (α=0.0-1.0) by atomistic molecular dynamics (MD) simulation. Our MD model approximates AgNP with a quasi-spherical silver nanocrystal with diameter 3.9 nm [2]. The united-atom force field G53a6 for PDMAEMA was used. We found that PDMAEMA adsorbs onto the AgNP surface through weak non-covalent interactions of their dimethylamino moieties. Our results demonstrate that the PDMAEMA adsorption onto AgNP depends strongly on its degree of protonation (Fig. 1*b*-*c*), as compared to conventional neutral polymers. Finally, we show that the pH-adaptive behavior of PDMAEMA keeps promising perspectives for their successful applications in novel generations of smart silver nanoparticles.

References

[1] D. Roy, J. N. Cambre, B. S. Sumerlin, *Prog. Polym. Sci.* **35**, 278-301 (2010)
[2] A. Kyrychenko, D. A. Pasko, O. N. Kalugin, *Phys. Chem. Chem. Phys.* **19**, 8742-8756 (2017)

5-4.P

STABILIZATION OF n-MOLECULAR HETERO-ASSOCIATE OF FLAVIN MONONUCLEOTIDE-THEOPHYLLINE IN AQUEOUS SOLUTION

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The water environment plays an important role in the processes of the association of aromatic compounds, in the formation of the native structure of DNA molecules, which are the target for antitumor antibiotics, and in the complexation of various small molecules with DNA. Aromatic biologically active compounds (BACs, ligands) include antitumor antibiotics, mutagens, carcinogens, some vitamins and food components. The investigation of hetero-association of aromatic ligands in neutral solutions is one of the important problems of molecular biophysics. Such studies provide a significant contribution to understanding the mechanisms of the medical and biological effect upon the combined use of several therapeutic drugs. In addition, hetero-association facilitates the increase of solubility of poorly soluble aromatic BACs in the presence of other aromatic molecules. Stable hetero-complexes are formed mainly due to interplanar interactions, which are determined by the π-interactions of the ring structures of chromophores, and the influence of the aqueous environment on hydrophobic ligand molecules.
Previous studies using nuclear magnetic resonance spectroscopy have shown that in aqueous solutions the molecules of the vitamin B_2 analogue flavin mononucleotide (FMN) and methylxanthine derivative theophylline (TPH) form stacked hetero-complexes [1]. To clarify the molecular mechanisms and structural features of the FMN-TPH hetero-complex, we obtained and analyzed the IR spectra of neutral D_2O solutions of FMN, TPH, and their mixtures. Also, a comparative study of the change in hydration of FMN, TPH and their complex was carried out using the piezogravimetry method. On the basis of the spectral changes, computer modeling of the hetero-complex made it possible to construct the spatial structure of the ***n***-molecular FMN-TPH hetero-associate.

References

[1] D. D. Andrejuk, A. A. Hernandez Santiago et al., *J. Mol. Struct.,* **889**, 229–236 (2008)

5-5.P

VISCOMETRIC RESEARCH OF THE COIL-SPIRAL TRANSITION IN AQUEOUS COLLAGEN SOLUTIONS

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Collagen is a body protein. This fact determines the relevance of the study of structural transformations occurring with collagen. The collagen molecule is a polymer chain, the units of which are amino acid residues of 12 types. Such chain can take different configurations, each has a definite value of potential energy. In its ground state, the collagen molecule is in the form of a spiral, and its potential energy is minimal.
In thermal motion, the configuration of the chain is constantly changing. At low temperatures, this motion is vibrational: atoms make small oscillations relative to positions corresponding to the ground state. Therefore, despite the existence of fluctuations, the configuration inherent in the ground state, on the average, is preserved. At high temperatures, thermal fluctuations increase. The configurations, in which the chain has time to fill, fill the area having the shape of the sphere. In this case, it is said that the chain is in the form of a coil. Changes in the shape of the chain, occurring with a decrease in temperature, are called the transition of “coil-spiral”.
Experimental measurements of the density and viscosity of aqueous collagen solutions of concentrations of 1, 2, 3, 4, 5 and 7 wt.% in the temperature range 303-353 K were performed. For describing the behavior of the viscosity of the solution, we introduce continuum model. By fulfilling this requirement, we will consider the coil as a sphere filled with a certain continuum, which consists of a chain and solvent molecules located in intervals between individual sections of the chain. This circumstance allows us to consider the mentioned region as a solid particle, surrounded by a liquid.
From the point of view of the mechanics of a continuous medium, the monospiar should be considered as a rod, and the coil-spiral transition – as a change in the shape of the particle. With these changes, the initial form of the particle is a coil, the finite – rod. Intermediate forms arise between these limiting cases. In this way, we arrive at a model that is a suspension of solid particles in the form of ellipsoids of rotation. Using the proposed model, it is shown that the number of spiral fragments increases with decreasing of temperature.

CELLULAR APPROACH TO VISCOSITY OF POLYVINYL ALCOHOL SOLUTIONS

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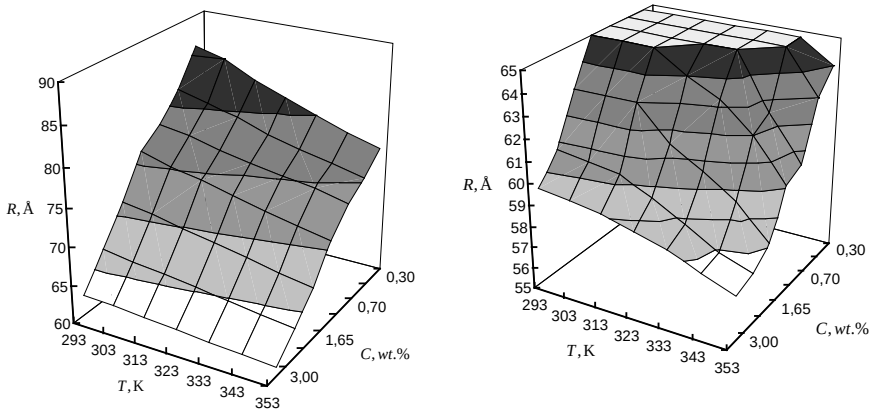
Experimental researches of the temperature dependences of the kinematic viscosity and density of polyvinyl alcohol (PVA) solutions in dimethyl sulfoxide ((CH3)2SO, DMSO) and water were carried out. In the researches, PVA Mowiol 6-98 (Kuraray) with a hydrolysis degree of 98.4±0.4 mol.% and without extra purification was used. The experiments were performed in the temperature interval 293-353 K and for PVA concentrations of 0.3, 0.5, 0.7, 1, 1.65, 2.32, and 3 wt.%. The kinematic viscosity was determined on capillary viscosimeters of the Ubbelohde type with an error of 2 %, by using standard techniques.

Figure 1. Effective radii of PVA macromolecules in DMSO (left figure) and water (right figure) as functions of the



temperature and concentration.

With certain reservations, macromolecular coils can be approximately considered as spherical particles consisting of a relatively hard core and a rarefied periphery [1]. The Malomuzh-Orlov formula allows the behavior of the viscosity of PVA solutions to be described in the macromolecule bulk concentration interval less than 0.5. The latter value, in essence, corresponds to the solution density, at which all macromolecules form contacts with one another [2].

The temperature dependences of the effective radii of PVA macromolecules in DMSO are shown to be linear within the experimental error limits. In aqueous PVA solutions, the temperature dependences of effective macromolecular radii are more complicated: at relatively low temperatures and concentrations, the effective radii of macromolecules remain unchanged; at higher concentrations, the effective radii decrease nonlinearly with the increasing temperature (fig 1). The concentration dependences of effective macromolecular radii have a nonlinearly decreasing character for both solvents.

References

[1] I.M. Lifshits, A.Yu. Grosberg, A.P. Khokhlov. *Usp. Fiz. Nauk* **127**, 353 (1979) (in Russian).
[2] O.V. Khorolskyi. *Ukr. J. Phys.* **62**, 858 (2017).

5-7.P

THE FEATURES OF STRUCTURE OF NANOCOMPOSITES BASED ON POLYETHYLENE GLYCOL AND ORGANOPHYLIC MONTMORILLONITE

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One of the most perspective nanofillers, which are used in polymer nanocomposites are clay minerals. Montmorillonite (MM) is inorganic filler with layered structure. Intercalating polymer in layered clay hosts can produce polymer electrolyte composites with huge interfacial area. The higher interfacial area reduces the crystallinity of PEO chains and sustains the mechanical property of semi-crystalline PEO based nanocomposites. The purpose of this work is to study the influence of the montmorillonite on the features of structure's forming of model systems based on polyethyleneglycol (PEG). The method of wide angle x-ray scattering (WAXS) with Debay-Sherrer geometry wase used for studying the influence of the nanofiller on polymer matrix in bulk. The method of WAXS with modify Bragg-Brentano geometry was used for studying the influence of the nanofiller on polymer matrix in the thin films, which were formed on the glass plate. The theoretical bases of this method were published in [1].

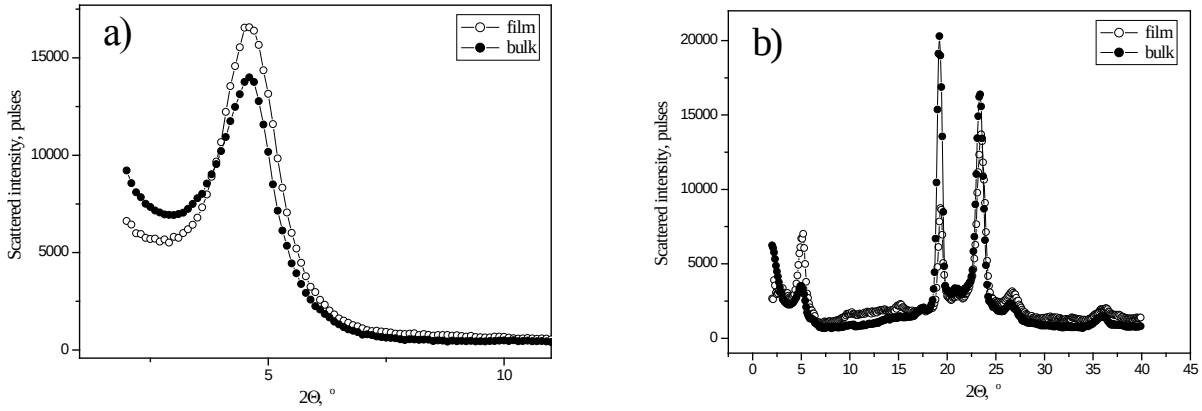

Fig. 1. WAXS curves of MM (a) and PEG+5% MM (b) in bulk and thin films.

It was established, that introduction of MM into the PEG matrix leads to the increasing of amorphous material of matrix material. In particular, the part of polymeric chain fragments intercalate into the interlayer space of organoclay, forming on each of internal surfaces, monolayer of the substantially straightened fragments of polymer molecules. As seen from fig.1a, the integral intensity of MM peak increases, when the MM was coated the plate. So, the glass plate has an oriental influence on MM. It was shown, that the degree of crystallinity of neat PEG-1000 decreases from 82,6% to 73,1%, when the thin film was formed. Forming the film leads to the limitation of conformations of PEG chains and the increasing of the part of amorphous material. The degree of crystallinity of nanocomposite PEG+5%MM decreases from 49,5% to 40,2%, when the thin film was formed (fig.1b). This phenomena can be explained by the forming in the nanocomposite based on PEG, complexes, which can be interpreted as the Lewis acid-base type interactions between silicate layers and the surface of glass plate [2]. These complexes limit the flaxibility of PEG chains, so the degree of crystallinity is decreasing [3].

References

[1] Yu.P. Gomza, V.V. Klepko, S.D. Nesin, E.A. Lysenkov, Yu.A. Kunitskiy, M. Yu. Barabash and L.G. Khomenko, *Nanosystems, nanomaterials, nanotechnologies* **7 (2)**, 411 (2009).
[2] H.W. Chen and F.C. Chang, *Polymer* **42**, 9763 (2001).
[3] E.A. Lysenkov, Yu. P. Gomza and V.V. Klepko. *Polym. J.* **32 (3)**, 223 (2010).

5-8.P

CD SENSING OF CONFORMATION'S ALTERATIONS OF SERUM ALBUMIN BY IRON (II) CLATHROCHELATES

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The conformational transitions of proteins usually affect their functions that cause an actuality of their exploring. Molecules gaining chirality upon their binding to proteins (i.e. giving response in circular dichroism (CD)-spectra) could possess high spectral sensitivity to such conformational alterations. The ability of cage metal complexes - iron(II) clathrochelates to induce a specific signal in visible range of CD-spectra upon the binding to protein was discovered. The most pronounced signal was observed for their complexes with serum albumins. The high binding affinity to bovine serum albumin (BSA) was shown for clathrochelates with carboxy groups. For hexacarboxy derivatives, the binding constants were 10^3-10^4 M^{-1}, binding ratio - 1-2 clathrochelate per protein molecule. Here we report that clathrochelate bearing six orthocarboxyphenyl groups is able to reflect by changes in CD-spectra alterations in protein structure (1) on "close structure" of serum albumins and (2) upon the protein conformational changes. The clathrochelate ability to discriminate human serum albumin from BSA by gaining CD-spectra of different shape was shown. Besides, conformational changes that albumins undergo upon pH variation were reflected by the changes of form, sign (negative/positive) and intensity of clathrochelate's CD-bands. That points out structure alterations of clathrochelate-albumin complex with pH variations. These alterations were confirmed by protein fluorescence quenching studies. The binding of clathrochelate to albumin resulted in decrease of protein intrinsic emission; it varied with pH (correspondingly BSA conformational transitions). The quenching was weak at pH 3.7 (in 1.5 times) - partially unfolded in domain III conformation and significant at pH 6 (in 14.6 times) – native form. We suggest the interest in further study of clathrochelates as reporters with CD sensitivity to proteins that are able to determine their conformational alterations.

The project leading to these results has received funding from EU Horizon 2020 research and innovation programme under Marie Skłodowska-Curie (grant-778245).

ABSORPTION, ELASTICITY PROPERTIES OF RADIATION CROSS-LINKED HYDROGEL, BUBBLE POLYSTYRENE AND ANISOTROPY PROCESSING AUTOMATED SYSTEM

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Bandages from the radiation cross-linked hydrogel (CLHG) show by itself elastic films with thickness $h = 2 \div 4 \cdot 10^{-3}$ m – transparent jelly sterile material, that with C = 85÷90% consists of distillate water. They can contain antiseptic, anaesthetic, haemostatic. The efficient operation of the filter with a filtering charge from cellular polystyrene granules to trap cyanobacteria was explained. The software is developed for the automated system of anisotropy parameters analysis.

The static elastic module E ≈ 147,3 KPa at compression, E ≈ 105,3 KPa at extension; elastic limit $\sigma_E \approx 38$ KPa, effective fluidity limit $\sigma_{fl} \approx 82$ KPa; strength limit at compression $\sigma_{st} \approx 145$ KPa for the radiation cross-linked hydrogel + 10% polyvinyl alcohol $(C_2H_4O)_n$ on fig. 1.

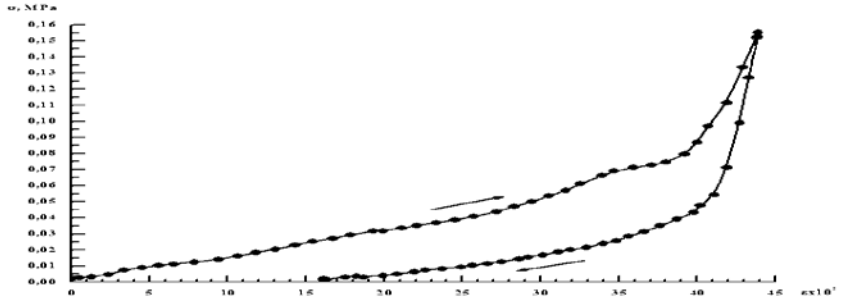

Fig. 1. Diagram of strain – deformation σ - ε of radiation cross-linked hydrogel + 10% polyvinyl alcohol $(C_2H_4O)_n$.

It is 3D polymeric net on fig. 2, fig. 3 - is the sponge with the pores size $d \leq 10^3$ nm, due to it contains distillate water, assumes the diffusion of solutions, but does not skip the bacteriums.

Fig. 2. Microstructure of radiation cross-linked hydrogel K 44.

Fig. 3. Microstructure of radiation cross-linked hydrogel C 44+Ag.

Conclusions

Thus, the optimum concentration C = 5% of polyvinyl alcohol $(C_2H_4O)_n$ radiation cross-linked hydrogel, bubble polystyrene with the maximal absolute values of the elastic limit σ_E; static elastic module E at compression, at extension; strength limit at compression σ_{st} in consequence of the formation of the polyvinyl alcohol molecules nanoclusters.

ABSORPTION PROPERTIES OF EXPANDED POLYSTYRENE, RADIATION CROSS-LINKED HYDROGEL AND PROCESSING AUTOMATED SYSTEM

A. P. Onanko*, D. V. Charny, Y. A. Onanko, S. A. Vyzhva, M. P. Kulish, O. P. Dmytrenko, T. O. Busko, L. I. Kurochka, O. I. Polovina

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The process of retention of phytoplankton on expanded polystyrene filtering loading was experimentally studied and its effectiveness was confirmed. Bandages from the radiation cross-linked hydrogel bandages for wounds for the grant of the urgent help at bleeding, burns must be biologically compatible and not stick to the wounds. The software is developed for the automated system of anisotropy parameters analysis.

The quasilongitudinal ultrasonic (US) velocity $V_{\parallel}$ = 504 m/sec, dynamical elastic module $E = \rho V_{\Updownarrow}^{2}$ = 15,24 MPa, "fast" quasitransversal US velocity $V_{\perp_1}$ = 280 m/sec, shear module $G = \rho V_{\Leftrightarrow 1}^{2}$ = 4,704 MPa, Puasson coefficient μ = 0,3532, specific density ρ = 60 kg/m^3 of expanded polystyrene are determined from the oscilloscopegramma on fig. 1,2.

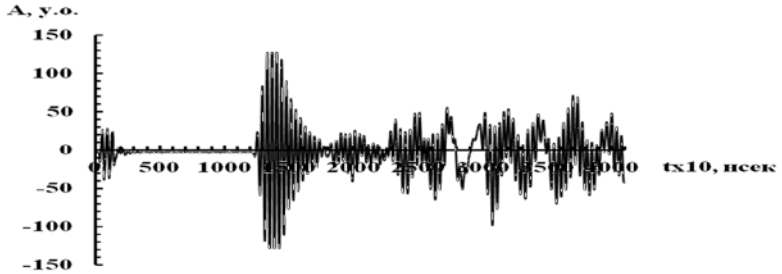

Fig. 1. Oscilloscopegramma of impulses with quasilongitudinal polarization $V_{\parallel}$ in expanded polystyrene.

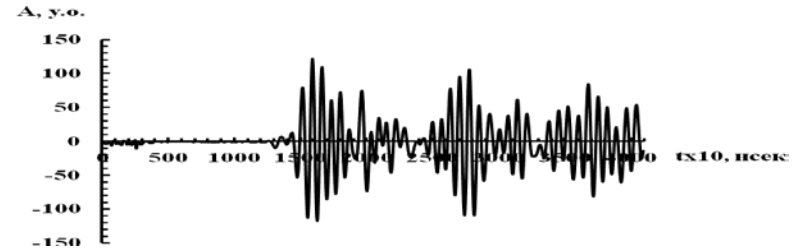

Fig. 2. Oscilloscopegramma of impulses with "fast" quasitransversal polarization $V_{\perp_1}$ in expanded polystyrene.

Conclusions

The decreasing of statical elastic module E at elastic module at compression, at extension; elastic limit σ_E; effective fluidity limit σ_{fl}; strength limit at compression σ_{st} of radiation sutured hydrogel, expanded polystyrene with increasing concentration polyvinyl spirit are discovered.

5-11.P

SPECIFIC BINDING OF POLYAMINES WITH DNA DOUBLE HELIX: A MOLECULAR DYNAMICS STUDY

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The interaction of natural polyamine molecules (putrescine, spermidine, and spermine) with the DNA double helix has been studied within the framework of molecular dynamics method. The goal of the study was to determine the most important binding sites of the polyamines with DNA and to characterize their impact on the double helix structure. To analyze the specific interactions of polyamines with DNA three systems consisted of the fragment d(CGCGAATTCGCGAATTCGCG) and polyamine molecule of defined type ($Putr^{2+}$, $Sprm^{3+}$ or Spm^{4+}) were simulated. The lengths of simulation trajectories were greater than 400 ns for each system. The obtained results show that all considered polyamine molecules tend to be localized in the minor groove of the double helix. Their residence time in the minor groove is within (10÷100)ns and increases as the charge of polyamine molecule increases. To analyze the influence of polyamine molecule on the structure of the double helix the widths of the minor and major groove were calculated. The results show that the width of the minor groove in the place of polyamine localization becomes narrower. The specificity of the polyamines to AATT nucleic base sequence was found. To determine the physical mechanism of the specific binding of polyamines with DNA the phenomenological model was developed. The estimations performed within the framework of the model show that the most energetically favorable place of polyamine localization is the groove of the double helix at the narrowest region. Since the narrowest groove is the minor groove at AATT nucleotide step the polyamine molecules are localized in that place. Thus, the specific interaction of polyamines with DNA is determined by the dependence of the groove width on sequence of nucleic bases.

5-12.P

EFFECT OF CARBON NANOTUBES ON POLYETHYLENE RELAXATION

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The focus of this work was to study the effect of multiwalled carbon nanotubes on relaxation processes in polyethylene. Several investigation techniques were used to achieve this objective. Nanocomposite materials were made from untreated multiwalled carbon nanotubes and low density polyethylene through a process of mixing and extruding. The filler content was varied from 0.5 to 5 vol.%. Changes in structure of composite induced by addition of carbon component were studied by X-ray diffraction method. The results of X-ray experiments showed an increase in crystallinity of the extruded composite matrix with increasing in multiwalled carbon nanotubes content. This is because of nucleating effect of nanotubes in the polymer matrix, causing more crystallization and orientation of molecules to take place around them.
Measurement of the amplitude dependences of internal friction was carried by the method of the inverse twisting pendulum. It shows that nanocomposite material on the base of polyethylene with multiwalled carbon nanotubes causes the structuring of the matrix and the relative stabilization of the segmental mobility of the molecular chains. The relaxation data showed that the material became more stiffness with the increase of the filler concentration to 5 vol.%.

5-13.P

VISCOELASTICITY OF GELATIN HYDROGEL AT LOW TEMPERATURES

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The molecular mechanism of viscoelasticity of gelatin hydrogel at low temperatures is studied. The gelatin (1480642, 2015, France) with bloom 200 is used. The temperature dependences of the shear modulus and the loss module of the gelatin hydrogel in the range 250-290 K were obtained by the method of torsion pendulum [1-2]. The presence of two relaxation regions, which correspond to the maxima of the loss modules is established. First region was located at a temperature of 254 K and a second region was located at a temperature of 268 K. It is shown that the first maximum caused by the mobility of the chains in the densely cross-linked areas of hydrogel networks. The second maximum caused by the rarely cross-linked areas in structure of the gelatin hydrogel. The changing of viscoelesticity of gelatin hydrogel at low temperatures is due to the fact that the melting of the hydrogel occurs above the melting of ice, namely at a temperature of 281 K is was established. The hypothesis about the presence in the system of densely cross-linked areas with slow-motion moving of bound water molecules is proposed.

References

[1] O.Yu.Aktan, *Functional Materials*, **16(2)**, 170-173 (2009).
[2] L.A.Bulavin, O.Yu.Aktan, *Advanched in Molecular Medisine*, **1(3)**, 103-106 (2005).

5-14.P

THE MEHOD OF DETERMINING THE DEGREE OF DISODER IN THE SYSTEM "BIOPOLYMER-SOLVENT"

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The method of determining the degree of disoder in the system "biopolymer-solvent" is proposed. For such system a biopolymer consists of two phases. These phases are ordered and disordered. A quantity of the disordered phase increases in time due to the inclusion of solvent molecules into the structure of the ordered system, namely swelling of the keratinous epidermis in water. The main calculated parameters in the proposed method are the time dependences of the diffusion coefficient and the time dependences of the shear modulus. These values are obtained from the experiment. The peculiarity of this model is that the keratinized epidermis is treated as an ordered "brick wall" model [1]. The structural unit of such model contains two components, namely the insoluble keratin granule and the lipid structures surrounding this granule. In the process of contact with water the volume of insoluble keratin granule remains stable. The space of lipid systems increases the volume due to the disordering of the chains in the entry of the water molecules. Thereby in the process of swelling in the regions of insoluble keratin the interaction with water is absent. The changes in the viscoelastic properties of the system are determined by the changes in the viscoelastic properties of the macromolecular structures surrounding the granule. The nature of disorder of the biosystem at the contact with water is described by the dimensionless coefficient. This value takes into account the changes of the structure in the zones of swelling.

References

[1] J.C.Weaver, T.E.Vaughan, Y.Chizmadzhev, *Advaced Drug Delivery Reviews*, **35**, 21-39 (1999).

RELAXATION AND STRUCTURAL TRANSITIONS IN GLUCOSE AT LOW TEMPERATURES

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The main goal of our study of glucose was to solve some problems in physics and medicine. These problems can be divided into two groups. The first group includes problems associated with the fact that glucose is one of the components of living organism. To solve these problems the behavior of glucose in the living organism is modeled using aqueous solutions of glucose as the model systems. The second group includes the problems associated with the manufacture of drugs in the form of tablets or powders, which contain glucose as the component. For them, the issue of preserving the quality of drugs with time is important, since glucose is known to be able to intensively absorb the moisture from the environment. Mentioned problems are based on the interaction of glucose with water, so the purpose of this work is to study the influence of water on the dielectric properties of glucose.

The temperature dependences of the complex permittivity for anhydrate and monohydrate glucose were obtained. On these dependencies, a relaxation process is observed at temperatures of 100-200 K for glucose anhydride, and this process is absent for monohydrate.

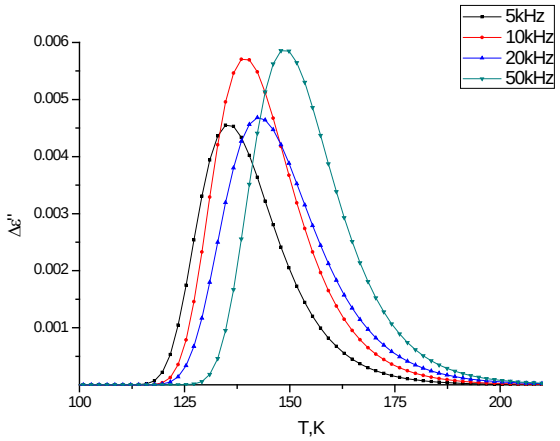

Fig.1 Temperature dependence of the imaginary part of dielectric constant $\Delta\varepsilon' = \varepsilon' - \varepsilon_0'$ at different frequencies

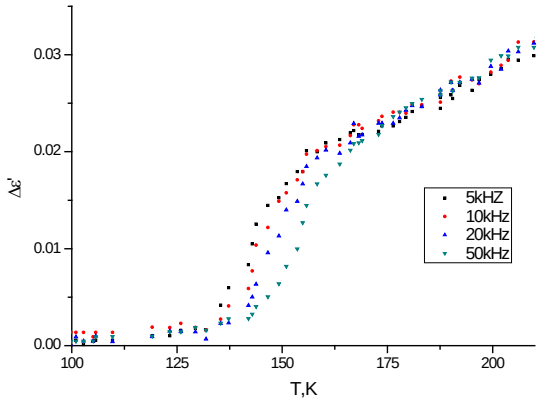

Fig.2 Temperature dependence of the real part of dielectric constant $\Delta\varepsilon'' = \varepsilon'' - \varepsilon_0''$ at different frequencies

In the one time relaxation approximation we calculated the activation energy $\frac{U}{k} = 29\text{к}J$, and the effective dipole moment $\frac{N\mu^2}{3k_B\varepsilon_0} = 193K$. using the ratio

$$\delta\varepsilon = \varepsilon_0 - \varepsilon_\infty = \frac{N\mu^2}{3k_B\varepsilon_0} \frac{exp\left(-\frac{V}{kT}\right)}{\left[1 + exp\left(-\frac{V}{kT}\right)\right]^2}$$

and the conditions of the maximum of the function ε(T): $\omega\tau_0 exp^{\frac{U}{kT}} = 1$.

We believe that the relaxation process may be related to the motion of methylol groups in the field of crystalline lattice defects.

5-16.P

INVESTIGATION OF THE FREQUENCY DEPENDENCE OF ELECTRICAL CONDUCTIVITY, DEPENDING ON THE TEMPERATURE OF THE AQUEOUS SOLUTION OF HYDROXYPROPYLMETHYL CELLULOSE

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Hypromellose is studied because of problems that can be divided into two groups. The first group includes problems associated with the fact that hypromellose has a unique property of thermal gelling: each type of substitution is characterized by its own gelation temperature. The second group of problems is connected with the creation of drugs in the form of tablets or capsules (namely, the shells for them), and hypromellose is a component of such shells. In particular, matrix tablets are made, which mainly consist of a drug substance and hypromellose.

Frequency and temperature dependences of electrical conductivity of hypromellose and NaCl-water system were obtained. These figures show a nonmonotonic dependence of the specific electrical conductivity on frequency, and this result are beyond the borders of our model (we suggest that . specific electrical conductivity of investigated system in the frequency range (0.1÷100)kHz does not depend on frequency.

For the purpose of studying the electrical properties (specific conductivity) of the electrolytes, the active components of the resistance at different alternating current frequencies are experimentally measured with the help of the automatic alternating current bridge P5083. A three-electrode capillary cell with platinum electrodes joins the bridge through the switching block. Also, the bridge through the controller connects to the computer. Thus, it is possible to automate the measurement process and write data into a file for further processing.

We calculate specific conductivity **κ**, using formula (1)

$$K=l_{12}/(S*(R_{13}-R_{23})) \qquad (1)$$

where **κ** – specific electrical conductivity, l_{12}- distance between electrodes 1 and 2, S – capillary cross section, R_{13} and R_{23} – the measured resistances, when bridge is connected to the electrodes 1,3 and 2,3 accordingly.

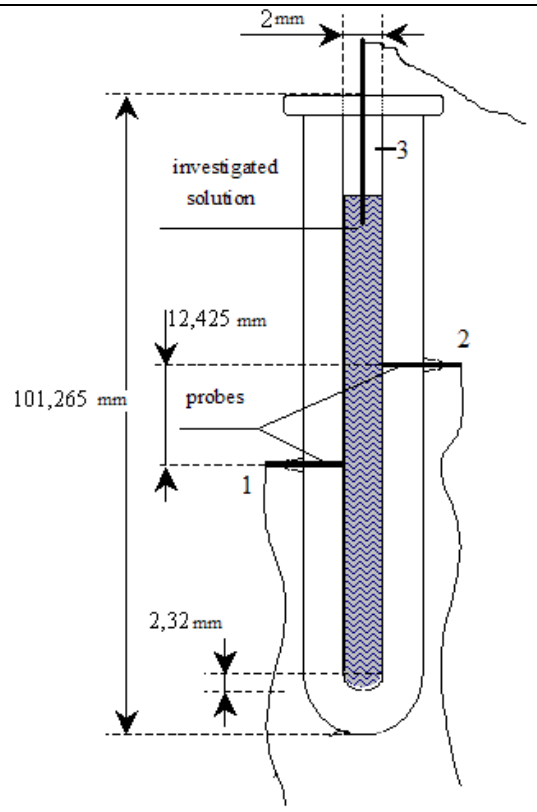

Fig.1 Capillary cell.

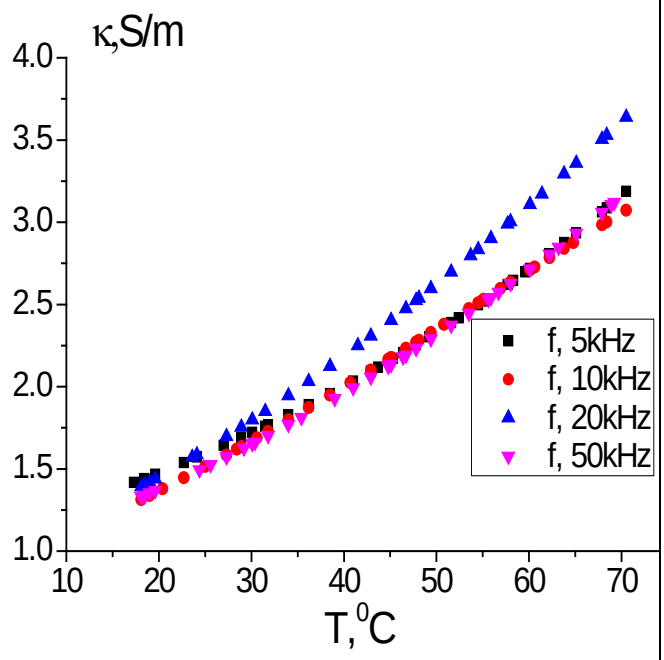

Fig.2 Frequency and temperature dependence of specific electrical conductivity of hyprometholose-NaCl-water solution (3%)

Section 6. Mixtures of Fullerenes and Nanotubes with Liquids

Oral session

6-1.O

COLLOID CHEMISTRY OF FULLERENES: HYDROSOLS, ORGANOSOLS, AND UNUSUAL 'MOLECULAR' SOLUTIONS

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This report is aimed to shed light on the nature of fullerene solutions in solvents of different nature. There are four main types of such systems formed by entire (non-modified) fullerenes, (i) aqueous colloidal systems, or hydrosols and suspensions; (ii) colloidal systems in polar organic solvents, or organosols; (iii) solutions in so-called good, or strong solvents, conceivably molecular solutions; (iv) solutions in so-called reactive solvents, in fact nitrogen-containing ones, which belong rather to systems with covalently modified fullerenes and thus are beyond the shape of the present report.

Nowadays, aqueous systems, especially hydrosols, are studied thoroughly. Despite different procedures of preparation and some peculiarities of properties, they turned out to be typical hydrophobic colloids, which obey the Schulze–Hardy rule and DLVO approach. Even the most complicated problem, the origin of the negative charge of species, is almost solved [1].

Though organosols are presently well-known, the studies of their interaction with electrolytes are few in number. However, even first results seem to be promising. The Hamaker constant of C_{60}–C_{60} interaction as determined basing on the data obtained using coagulation of organosols coincides with that obtained from examining the hydrosols. The origin of the negative charge of colloidal species in acetonitrile is probably the formation of fullerene anion-radicals. Overcharging of colloidal species by means of metal cations and H^+ ions takes place in methanol, acetonitrile, its mixtures with benzene and toluene [2, 3].

Finally, most enigmatic are probably the fullerene solutions in good solvents, such as benzene, toluene, xylenes, CS_2, etc. These solutions are usually considered as molecular ones but demonstrate dualistic behavior and properties, as studied via various experimental methods. To explain the reason of this uncertainty, a concept of periodic colloidal systems should be proposed. In this case, each C_{60} molecule covered by a thick solvation shell may be considered as a colloidal particle.

References

[1] N. O. Mchedlov-Petrossyan. *Chem. Rev*. **113,** 5149–5193 (2013).
[2] N. O. Mchedlov-Petrossyan, N. N. Kamneva, Y. T. M. Al-Shuuchi, A. I. Marynin, O. S. Zozulia, A. P. Kryshtal, V. K. Klochkov, S. V. Shekhovtsov. *PCCP* **18,** 2517–2526 (2016).
[3] N. O. Mchedlov-Petrossyan, Y. T. M. Al-Shuuchi, N. N. Kamneva, A. I. Marynin, V. K. Klochkov *Langmuir* **32,** 10065–10072 (2016).

SPECIFIC FEATURES OF FULLERENES IN BINARY MIXTURES: NEW OPPORTUNITIES FOR BIOMEDICINE

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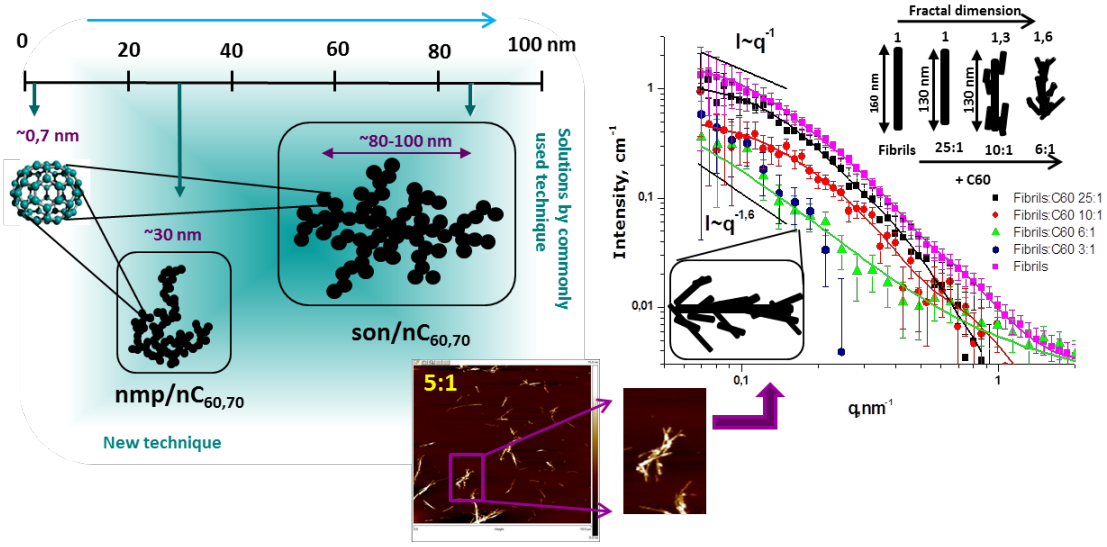
The increase in the applications of fullerenes in various fields including electronics, optics, cosmetics, and pharmaceutics raises the requirements for control of dimensions of the fullerene aggregates in various solvents. First of all, this concerns solutions in polar solvents and their mixtures, due to low fullerene solubility in them. Dissolution and equilibration of fullerenes in solvents is a complex kinetic process accompanied by various effects, such as the unexpected aggregation in solvents with good fullerene solubility or solvatochromic shifts in absorption spectra [1,2]. Despite numerous papers devoted to fullerene dispersions the behavior of fullerenes is still unclear upon transition from an organic solvent to a polar environment [3].

The work concerns the problem of aggregation of fullerenes in various systems and accompanying effects. The changes in the UV-Vis spectra observed when varying the solvent mixture composition are discussed. The interesting fact discovered is that solvatochromism as well as the cluster size of fullerenes strongly depend on the order of the mixture preparation. As a result, a new method of fullerene dissolution in water was suggested. The obtained aqueous solution of fullerenes C_{60} and C_{70} are characterized by the small size of the fullerene aggregates, in comparison with the solutions synthesized by the previously known techniques. The new solutions show a low toxicity and, according to SANS data, effectively destroyed amyloid fibrils, which responsible for neurodegenerative Alzheimer's and Parkinson's diseases.



References

[1] O.A. Kyzyma, T.O. Kyrey, M.V. Avdeev, et al. Chem. Phys. Lett. 556 (2013) 178.
[2] Nagorna T.V., Kyzyma O.A., Chudoba D., et al. J. Mol. Liq. 235(2017)111.
[3] N. O. Mchedlov-Petrossyan, Chem. Rev. 113 (7) (2013) 5149.

INFLUENCE OF WATER ON ADSORPTION OF SIMPLE MOLECULAR ANIONS BY NANOSTRUCTURED CARBON MATERIALS

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Increasing pollution of heavy metals in groundwater and surface water effectively reducing the supply of freshwater for human use. The hexavalent chromium Cr(VI) ions are typical heavy metal ions in waste water. Chromium can exist in water as dichromate ($Cr_2O_7^{2-}$), hydrogen chromate ($HCrO_4^{2-}$), and chromate molecular anions (CrO_4^{2-}). Carbon nanostructured materials have been intensively studied at present as materials for efficient removal and storage of various toxic molecules. Some studies have already indicated that functionalized CNTs are promising for the removal of the toxic heavy metals from water wastes. Theoretical modeling of such molecular adsorption on the CNTs surfaces provides understanding of adsorption mechanisms.

The adsorption characteristics of the chromium molecular oxyanions on the surface of pristine and N/B-doped and functionalized CNTs were computationally studied in this work. The geometry - optimized calculations of the electronic structure of CNTs with adsorbed chromium molecular oxyanions were carried out within molecular cluster approach by Gaussian 09 program package [1]. Influence of water surrounding on adsorption characteristics was taken into account within polarizable continuum model (PCM).

Binding energies, relaxed geometries and charge difference of chromium molecular oxyanions in adsorbed and free states were calculated and analyzed. Adsorption mechanism was illustrated by dependence of the binding energy on the tube - molecule oxyanions distances. Calculation results were discussed in view of potential application of the CNT-based materials as efficient adsorbents of toxic hexavalent metals oxides in water surrounding.

References

[1] M.J. Frisch, G.W. Trucks, H.B. Schlegel, et al. Gaussian 09 (Gaussian, Inc., Wallingford, CT, 2009).

KINETICS OF FULLERENE C_{60} AGGREGATION IN POLAR LIQUIDS AND THEIR MIXTURES WITH WATER

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Fullerenes, a new allotropic form of carbon discovered at the end of last century, provoke much interest partly due to their ability to dissolve in various liquids and the interesting effects that occur in their solutions [1]. These effects include clusters formation and growth, solvatochromism and some others.
The present report is dedicated to theoretical and experimental investigation of fullerenes aggregation in polar solutions. Slow growth of large fullerene clusters has been reported to occur in these systems [2]. It is supposed to be connected with formation of charge-transfer complexes between fullerene and solvent molecules [3]. We consider novel experimental data for C_{60}/N-methyl-pyrrolidone (NMP) solution, including DLS and UV-Vis kinetic measurements. For theoretical description of aggregation a model system similar to C_{60}/NMP is considered and the approach based on kinetic theory of nucleation has been developed. The cluster-size distribution functions within the model of limited growth are obtained for the whole period of systems evolution.
Using the developed approach we also consider the critical effect of cluster decomposition in C_{60}/NMP solution, that occurs after water addition to the system [4]. This effect may be used in the future for obtaining of fullerene-water solutions with given properties for biomedical applications. The possible models for description of the effect are discussed.

References

[1] Avdeev, M.A., Aksenov, V.L., Tropin, T.V., Models of cluster formation in solutions of fullerenes, *Russ. J. Phys. Chem. A.*, **84** 1273-1283 (2010).
[2] Nath, S., Pal, H., Sapre, A.V., Effect of solvent polarity on the aggregation of C60, *Chem. Phys. Lett.* **327** 143–148 (2000).
[3] Kyzyma, O.A., Korobov, M.V., et al., Aggregate development in C60/NMP solution and its mixture with water as revealed by extraction and mass spectroscopy, *Chem. Phys. Lett.* **493** 103–106 (2010).
[4] Aksenov, V.L., Avdeev, M.V., Tropin, T.V., et al., Formation of fullerene clusters in the system C60/NMP/water by SANS, *Phys. B Condens. Matter.* **385–386** 795–797 (2006).

6-5.O

GENERATION OF SILVER NANOPARTICLES IN A PLASMA-LIQUID SYSTEM WITH A SECONDARY DISCHARGE

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Production of nano-materials with different nature, like carbon, non-metallic or metallic nanoparticles in plasma systems is one of the perspective directions of plasma technology. The noble metal nanoparticles (silver especially) has wide application in medicine: sterilization, healing acceleration and stabilization of bactericidal ointments. One of the effective methods to produce such particles is the processing of these metals salt colloidal solutions using electric discharge. The plasma-liquid system with secondary discharge that supported by rotating gliding discharge can be used for this task. The interest to systems with rotating gliding discharge is caused because such discharge allows to obtain non-equilibrium atmospheric pressure plasma with large cross section. This provides a large contact area between the plasma and the treated liquid. A potential jump created by a secondary discharge above the liquid surface provides more efficient penetration of active particles from plasma into the liquid.

The secondary discharge is maintained between the liquid surface and the channel of self-sustained discharge (SSD). Rotating gliding discharge (RGD) is used in this system as the SSD. The plasma-forming gas was supplied in the discharge chamber through two supply channels tangential to the inner cylindrical wall of the reaction chamber. The working liquid was placed below RGD in a glass vessel. The electrical potential is transferred to the liquid through the electrode at the bottom of the vessel. For the generation of discharges, DC and AC power supplies were used. Solution of $AgNO_3$ with addition of different concentrations of surface-active substances was used as a working liquid.

Parameters of liquids after plasma treatment were investigated by absorption spectroscopy method.

The Atomic Force Microscope and Dynamic Light Scattering measurements were used to determine the particle sizes obtained during the processing.

The sizes of nanoparticles measured a few days after processing were from tens to hundreds nanometers.

6-6.O

OPTICAL PROPERTIES OF NANOFLUID OF O-XYLENE / FULLERENES C_{60}

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Molecular solutions of fullerenes in oils and aromatic hydrocarbons are characterized by high stability – do not aggregate or sediment with time. The additives of fullerenes in base fluids insignificantly affect the viscosity and lead to an increase in the heat capacity and thermal conductivity. These properties of fullerene solutions in aromatic hydrocarbons determine the feasibility of developing a new generation of coolants for direct absorption solar collectors.

To assess the feasibility of using molecular solutions containing fullerenes for use in alternative solar energy, it is necessary to have information about their optical characteristics. In this respect, the most important are data on the light absorption in the visible wavelength range.

In this work, molecular solutions of fullerenes C_{60} in o-xylene are considered as the research objects. o-Xylene was chosen as the base fluid, since fullerenes C_{60} are good soluble in it.

The main aim of this work was to study optical properties of fullerenes C_{60} solutions as a function of concentration. Measurements were performed on a Shimadzu-1700 spectrophotometer in the concentration range 0.08-0.74 wt.% of fullerenes C_{60} at the temperature 18°C in the wavelength range of 300-1100 nm. The obtained dependences of the absorption spectra of fullerenes C_{60} solutions on the wavelength of the radiation show a nonlinear absorption character, similar for all solutions (concentrations 0.08, 0.23, 0.55 and 0.74 wt.%). Each dependence has several absorption peaks, the position of which depends on the concentration of the solution, and one common for all samples absorption minimum at approximately 440 nm. In addition, for all samples, a sharp decrease in the light absorption in the wavelength range of 620-700 nm and complete optical transmittance at wavelengths from 700 nm and more are observed. On the basis of the obtained experimental data, conclusions regarding the physical nature of the nonlinearity of the optical properties of the studied o-xylene / fullerene C_{60} solutions are formulated.

6-7.O

CARBON NANOTUBES IN WATER SUSPENSION WITH DNA: PHOTOLUMINESCENCE ENHANCEMENT INDUCED BY ANTIOXIDANT GLUTATHIONE

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Individual single-walled carbon nanotubes (SWNTs) in water suspensions display photoluminescence (PL) which quantum yield can be increased by addition of reducing agents including thiol compounds, most likely due to passivation of quenching defects [1]. In the present report the influence of antioxidant glutathione on nanotube PL was studied and compared with other thiols: cysteine, dithiothreitol (DTT), dithioerythritol (DTE). Steady aqueous suspensions of SWNTs with single-stranded DNA (ssDNA) were prepared with sonication for 30 or 90 min resulting in different SWNT biopolymer coverage [2]. PL spectra of suspended SWNTs were registered at gradual addition of glutathione or other thiols (up to 10^{-3} M). Obtained dependencies of normalized PL band integral intensity on logarithm of concentration (concentration curves) have shown that all thiol compounds studied caused different increase of PL bands corresponding to various SWNT chiralities. This was more pronounced in case of 90 min-sonicated suspension and ratiometric sensing technique involving the change of two resolved bands intensities ratio was proven applicable for glutathione, giving ~$5 \cdot 10^{-6}$ M level of detection. Concentration curve obtained for glutathione was shifted towards higher concentration by an order of magnitude comparing to cysteine despite rather similar redox properties. The shift can be caused by peculiarities of cysteine and glutathione reduced and oxidized forms interaction with SWNT sidewall [3]. The results obtained for glutathione, cysteine and isomers DTT and DTE revealed tendency that stronger reduced yields larger PL increase and provided evidence that redox properties in the vicinity of SWNT are crucial for this effect.

References

[1] A.J. Lee, X. Wang, L.J. Carlson, J.A. Smyder, B. Loesch, X. Tu, M. Zheng, T.D. Krauss, *Nano Lett.*, **11**, 1636–1640 (2011).
[2] N.V. Kurnosov, V.S. Leontiev, V.A. Karachevtsev, *Nanoscale Research Lett.*, **11**, 490-497 (2016).
[3] A. Hirano, T. Kameda, S. Sakuraba, M. Wada, T. Tanaka, H. Kataura, *Nanoscale*, **9**, 5389-5393 (2017).

6-8.O

LIQUID CRYSTAL DISPERSIONS OF ANISOMETRIC NANOPARTICLES: SPECTROPHOTOMETRY AND DIFFERENTIAL SCANNING CALORIMETRY STUDIES

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Complex liquid systems based on liquid crystals (LC) as anisotropic dispersion medium with micro- and nanoparticles of different nature more or less homogeneously distributed therein are nowadays a “hot” subject of research. Such systems are promising for many possible applications, and they are highly interesting objects from the viewpoint of modern liquid matter physics. One of fundamental questions is how different character of the nanoparticle (NP) anisometry can affect the observable properties of LC+NP dispersions. In this report, we summarize the results of our studies on LC matrices containing carbon nanotubes (rod-like), exfoliated particles of laponite (disc-like), spherical nanoparticles of diamond, particles of aerosil that can aggregate forming structures of different geometries, etc. A certain point of novelty is that we carried out comparative studies of all these systems in similar experimental conditions using similar measurement procedures and the same equipment. Our main attention was paid to optical spectrophotometry (dependences of optical transmission on temperature with a highly specific “transmission jump” at the nematic to isotropic phase transition) and differential scanning calorimetry (changes in location and shape of the phase transition peak in the heating and cooling modes). Taking into account the available literature data, possible generalizations and implications are discussed.

Poster session

6-1.P

SYMMETRIES OF HEAT-MASS TRANSFER AND HYDRODYNAMICS OF NANOFLUID AND THEIR HYDRODYNAMIC INSTABILITY

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Fluid flow, heat and mass transfer equations for nanofluids in parabolic approximation were investigated using their symmetries (Lie groups). On the basis of these symmetry groups self-similar forms for independent variables and functions were derived, which describe velocity, temperature and concentration fields. Therefore these self-similar forms and Buongiorno model enabled obtaining generalized system of self-similar differential equations for parabolic flows of nanofluids. In Buongiorno model physical properties of nanofluids (viscosity, thermal conductivity, diffusion coefficients and density) were specified in general form as functions of the temperature and nanoparticle concentration. Thus this self similar system has universal character because this system is free from any specific form of the functional dependence of the physical properties of nanofluids on the temperature and nanoparticle concentration. The self-similar system takes into account different additional effects that arise in nanofluid flows, particularly thermophoresis diffusion and Brownian diffusion. These two types of diffusion are important since their interaction controls the processes of heat and mass transfer in nanofluids. On the basic on proposed model the specific cases of heat of mass transfer for nano-fluids are considered. In particular, processes with film boiling and bioconvection are considered. Also on the basis of renormalization group analysis relation for the turbulent viscosity of the nanofluid flow is obtained. To create nanofluids and keep their properties preserved and stabilized, one can involve different methods, such as the centrifugal method. That is why centrifugal instability of nanofluid flow was investigated.

6-2.P

CRYSTALLIZATION BEHAVIOR OF LAPONIT − TRIPHENYL PHOSPHITE NANOCOMPOSITE

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Triphenyl phosphite [TPP, $P(OPh)_3$] is a simple molecular liquid at room temperature [1]. The cylindrical nanoparticles of laponite resemble plates with a diameter of approximately 25 nm and 1 nm thickness [2]. To create TPP/laponite nanocomposite to liquid TPP (1 cm^3) the powder laponite with mass of 0.3 g was added.
Results presented here show that, the interaction between the liquid TPP and laponite nanoparticles gives rise to a new crystalline phase with new properties. Namely, in addition to the already known stable crystalline phase of TPP whose crystallization occurs at 240 K (melting point 295 K) and metastable crystalline phase whose crystallization occurs at 260 K (melting point 291.6 K) [3], the nanocomposite of the clay nanomaterial laponite and TPP can crystallize at room temperature in another crystalline phase. The new phase of composite melts higher the stable phase of TPP, i.e. at 310 K. Differential scanning calorimetry results were complimented by the IR spectroscopic investigation of the structural changes during the crystallization processes in TPP/laponite nanocomposites in the 400-4000 cm^{-1} spectral range.

References

[1] I. Cohen, A. Ha, Z. Zhao, M. Lee, T. Fischer, M. Strouse, D. Kivelson, *J Phys Chem*., **100,** 8518-8526 (1996).
[2] M. Fatnassi, M. Es-Souni, *Royal Society of Chemistry,* **5,** 21550-21557 (2015).
[3] J. Baran, N.A. Davydova, M. Drozd, *The J. Chem. Phys*., **140,** 104512-6 (2014).

LIQUID AND GRANULAR STREAMS, MANIPULATED BY EXTERNAL INHOMOGENEOUS ELECTRIC FIELD

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We study theoretically and experimentally motion of liquid droplets and granular beads generated by inhomogeneous electric field.
Nevertheless, both systems has completely different origin, they shows an isomorphic behavior on macro-scale, when being subject into inhomogeneous external electric field. It has been found that under the appropriate values of internal parameters (liquid, or grain sizes and weighs and their material properties) and the bias of external field in both cases we observe formation of stream motion with a particular dynamics. Theoretical interpretation of that fluid jet has been done by use of dielectrophoretic argumentation developed in [1]. Also, levitation criteria which corresponds to particular stream dynamics [2] has been theoretically discussed and recommended to be experimentally checked.
The phenomena has been studied experimentally in forms of horizontal liquid drop stream injected from capillary tube and vertical granular cluster jet both subjected into gravity in the presence of inhomogeneous electric field. In both experiments, we observe existence of stream velocities saturation effects, which reflect the balance between the inertia (gravity) effects and electrophoretic effects due to external electric field inhomogeneity.
We outline a numerous practical applications of the discovered effects such as for dust evacuation and electrophoretic technologies.

References

[1] Aliotta, Francesco, Oleg Gerasymov and Pietro Calandra. "Electrospray Jet Emission: An Alternative Interpretation Invoking Dielectrophoretic Forces." Intelligent Nanomaterials, p.51-90 (2016)
[2] Dolinsky, Yu, and T. Elperin. "Levitation and oscillations of neutral particles in a constant electric field." Journal of Applied Physics, 109, 114902 (2011)

AGGREGATION OF FULLERENE IN MIXTURES OF "GOOD" AND POLAR SOLVENTS: C_{60} IN TOLUENE–METHANOL SYSTEM

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The fullerene C_{60} readily forms colloidal solutions in methyl alcohol with more or less content of toluene. The UV absorption spectra in toluene – methanol mixed solvent even in 50 vol % alcohol resemble that in the aromatic 'good' solvent, whereas the system is already a colloidal one. This indicates that the C_{60} molecules associate being rather firmly solvated by toluene.

The properties and the aggregation processes of C_{60} in toluene–methanol mixtures were studied within the range of fullerene concentrations from 4×10^{-7} to 4×10^{-5} M. The threshold composition of the mixed solvent, which corresponds to the disappearance of single C_{60} molecules, has been found. An example of spectra (Fig. 1a) and results of dynamic light scattering (Fig. 1b) is shown below.

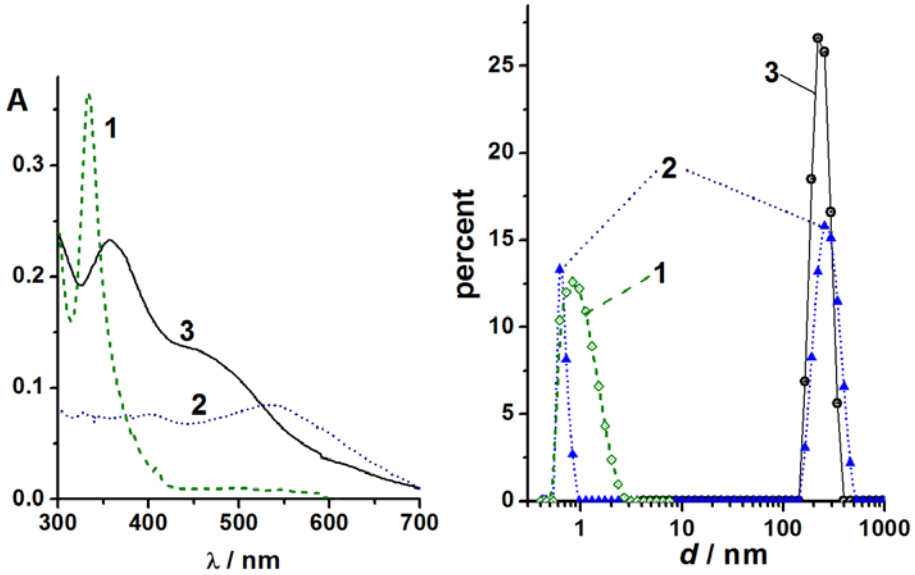

Figure 1 (a) UV-visible absorption spectra of C60 sol in methanol–toluene mixed solvents with methanol fraction of 30 vol % (1), 90 (2), and 99 vol % (3), optical path 1.00 cm; (b) the size distribution by intensity from DLS measurements – in 30 % methanol (1), in 90 % methanol (2), and in 99 % methanol. Fullerene concentration 6.0×10–6 M, measurements were made at 25 oC.

6-5.P

NEUTRON REFLECTOMETRY STUDY OF STRUCTURE AND GLASS TRANSITION IN THIN FILMS OF POLYSTYRENE-FULLERENE NANOCOMPOSITES

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Thin polymer films have numerous technological applications in various industrial and biomedical sectors related to protective and functional coatings, non-fouling biosurfaces, biocompatibility of medical implants, separations, advanced membranes, microfluidics, sensors, devices, adhesion, lubrication and friction modification[1]. In many cases, the films can be of complex composition with different types of polymers with complex architecture and other components such as nanoparticles. Polymers in thin films and nanocomposite structures can exhibit unusual physical properties due to the geometric constraints imposed by the presence of surfaces and interfaces. Polystyrene-fullerene films present a suitable model system for investigation of these properties. Neutron reflectometry has proved to be an effective method for studying PS/C_{60}, allowing evaluating the structural peculiarities of nanoparticles ordering in the polymer matrix [2].
In the present work, we performed neutron study of structure and glass transition in the thin films of polystyrene-fullerene C_{70} nanocomposite. PS/C_{70} and *d*PS/C_{70} solutions in toluene were spin-coated on Si (111) at 2000 rpm after filtering through 0.22 Milipore filter. Series of thin films samples with different concentration of C_{70} were prepared and investigated for the internal structure and glass transition.
Neutron measurements of polymer thin films in the temperature range up to 130°C were performed at the GRAINS instrument of the IBR-2, JINR. For this purpose, a special cell for samples was designed and created. Changing of the glass transition temperature has been observed and possible internal structure of films has been analyzed.

References

[1] E.Slaver. *Polymer Thin Films*, 304 (2016).
[2] Yaklin, M. a., Duxbury, P. M., & Mackay, M. E. (2008). Control of nanoparticle dispersion in thin polymer films. *Soft Matter*, *4*(12), 2441.

FLUID FLOWS IN MICROPOROUS AND NANOPOROUS FILTERS

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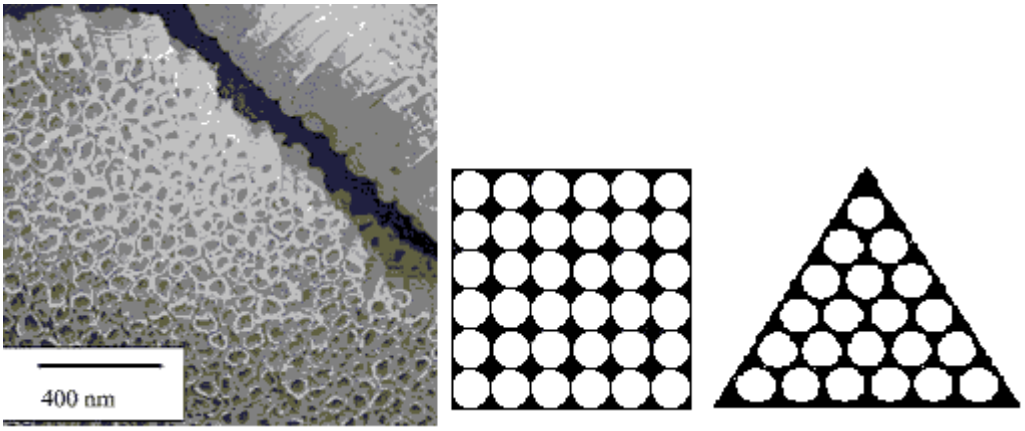
During the last decades a significant attention has been paid to micro and nanofluidic systems in which small amounts of technical or biological fluids move through the systems of tubes with diameters d=10-500 nm (nanofluidics) or d=10-500 mcm (microfluidics). The units for fluid purification/mixing, liquid heaters/coolers, fuel cells, microrobots, lab-on-a-chip devices and different microelectromechanical systems are based of flows of suspensions of nano/micro particles. As it was shown in numerous experiments, the volumetric rate in micro/nanofluidics is higher and the wall shear stress, dissipation and entropy production are lower that it is predicted by classical Poiseuille or Darcy laws [1].
In this study the steady flows of micro/nanofluids through the micro/nanoporous filters at a constant pressure drop are considered. The filters are modeled as a bundle of tubes (Kozeny-Karman model). The incompressible Navier-Stokes and heat transfer equations are solved with velocity slip and temperature jump boundary conditions at the walls. Material parameters for the fluid viscosity, density, specific heat, heat conductivity, and slip coefficients have bee taken from technical liquids and some biofluids (blood plasma, blood).
The generalized Kozeny-Karman formula for the micro/nanofluids is obtained. Numerical computations of the volumetric flow rate, heat flux and entropy production revealed the ranges for the model parameters when flow rate increase in 50-80% for microporous and in 10^2-10^4 times for nanoporous filters. The computational data correspond to the experimental measurements [2] on different micro/nanofilters.



a b

Fig.1. The nanoporous filter [2] (a) and its model with cubic and hexagonal arrangements of tubes (b).

References

[1] V. Cherevko and N. Kizilova, Nanophysics, Nanomaterials, Interface Studies, and Applications, Springer Proc. in Physics,183, 207–230 (2017).
[2] O. Bakajin, A. Noy, F, Fornasiero, et al., Nanotechnology Applications for Clean Water, 77-93 (2009).

MODIFICATION OF FULLERENE C_{60} BY PECTIN TO IMPROVE THE SELECTIVITY OF THE EFFECT ON THE CANCER CELLS: STRUCTURE INVESTIGATION

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Pectins, as a compound, are linear polysaccharides composed primarily of D-galactopyranosyluronic acids joined via α (1 4) glycosidic linkages. D-galacturonic acid content is important to the gelling capabilities of given pectin. Pectin has the anti-adhesive properties and can increase apoptotic responses of tumor cells to chemotherapy by inhibiting galectin-3-apoptopic function. Due to its anti-adhesive, apoptosis-promoting, and apoptosis-inducing properties, pectin is capable of targeting multiple critical rate-limiting steps involved in cancer metastasis. In addition, by inhibiting Gal-3 anti-apoptotic function and enhancing apoptosis induced by cytotoxic drugs, it holds the potential to increase dramatically the efficiency of a conventional chemotherapy [1]. In the other side, pectin can increase the bioavailability of the medicine in oncology treatment because of similar structure of pectin to glucose (in the cancer cells observe the increased uptake of glucose [2]). It should be noted that fullerene C60 and its derivatives are used also as anti-tumor drugs with the pleiotropic activity but unfortunately without selective action. For this reason, we use pectin as a fullerene transporter in the target cell.

In this research, we considered the possibility of gel-formation pectin matrix around fullerene by SANS, DLS, UV-spectroscopy and created primal theoretical model for understanding the mechanism of interaction fullerene C60 and poly-D galacturonic acid. The results indicated that pectin encapsulates of fullerene aggregates (Fig.1).

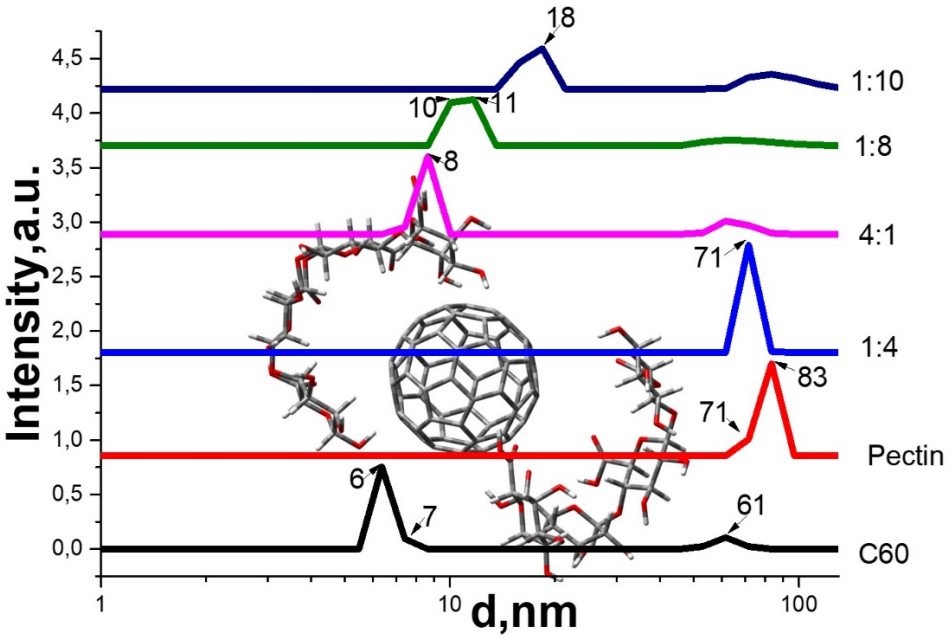

Fig.1 The DLS data of water solutions: C60, Pectin, C60 : Pectin.

References

[1] Modified citrus pectin anti-metastatic properties: one bullet, multiple targets [V.Glinsky, A.Raz //Carbohydrate Research 344 (2009) 1788–1791

[2] Biology of glucose metabolization in cancer cells A. Fadaka , B. Ajiboye, O. Ojo et all // Journal of Oncological Sciences 3 (2017) 45-51.

6-8.P

THEORETIC AND EXPERIMENTAL STUDY ON TITANIA NANOTUBE DOPED WITH AG METAL IONS

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The electronic state density and energy bands of Ag-doped anatase TiO_2 were studied by WIEN2k software package basing on DFT. The calculation results showed that the band-gap of anatase titania became bigger after doping with Ag metal ions, the band-gap transfers from 2.04 to 2.5 eV, but a new energy band appeared among the forbidden band after the Ag atoms substitution, the interband width of Ag-TiO_2 is 0.17 eV, which is located at -0.07 eV; more excitation and jump routes are opened for the electrons, the lowest excitation energy can achieve 1.2 eV, which may allow the photons with lower energy (at longer wavelength, such as visible light) to be absorbed. Ag ions were implanted into the titania nanotube sample by MeVVA(Metal Vapor Vacuum Arc) implanter, the photo-electrochemical response and photo-degradation experiment of titania nanotubes samples implanted with Ag ions were tested under UV and visible light; the results indicated that the performance of implanted titania naotubes were enhanced both under UV and visible light; it is worth mentioning that the photo-current density could reach 0.145 mA/cm^2 under visible light, which is 181 times higher than those of pure TiNT, and the k value of degradation Methyl Orange can obtain 0.30 h^{-1}, which is 71 times higher than those of pure Ti nanotube. All the experimental results are consistant well with the theoretical results.

Keywords: WIEN2k ; Density function theory; TiO_2 nanotube; Ag ions doped

6-9.P

IMPACT OF SURFACTANTS AND CLAY PLATELETS ON ELECTROKINETIC POTENTIAL AND SIZE DISTRIBUTION IN CARBON NANOTUBES AQUEOUS SUSPENSIONS

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Stabilization of aqueous suspensions of carbon nanotubes (CNTs) is an acute task for a number of technological applications. The effects of surfactant (CTAB, cationic surfactant and Triton X-100, non-ionic surfactant) and clay platelets (Laponite RD® (Lap)) on the electrokinetic potential and aggregation stability/size distribution of CNTs have been studied. The studies were performed at constant pH (4.5±0.1), different concentrations of surfactants and different mass ratios X=Lap/CNTs. The effects of aging time and duration ultrasonic treatment were also investigated. The procedure of preparation of mixed Lap/CNT+CTAB suspensions has no effect on the stability and electrokinetic properties. For concentration of CTAB in the interval of C_s=$3.64\cdot10^{-5}$–$1.82\cdot10^{-2}$ wt % a narrow monomodal size distribution of aggregates with median size of 21–24 μm was observed. At higher CTAB concentrations (above critical micelle concentrations, CMC), formation of aggregates with median size of 140-150 μm takes place, with preserving the monomodal size distribution. Aggregation of CNTs in this case probably occurs by deposition of individual CNT on the surface of primary aggregates. Addition of Lap platelets in the range from X=0 to 0.4 causes a monotonic decrease of the ζ-potential of the CNTs from -40 mV to -30 mV with reaching its plateau value at $X\geq0.4$. This evidences the high surface coverage of CNTs by Lap platelets at which the CNT+Lap complex acquires the ζ-potential value of Lap. In mixed Lap/CNT suspensions (X=1.0), a bimodal particle size distribution was registered, with appearance of big aggregates (≈150-300 μm), both in dilute (C_s=$3.64\cdot10^{-5}$–$3.64\cdot10^{-3}$ wt %) and concentrated (C_s>C_s^{CMC}) solutions. These big hybrid Lap/CNT aggregates were loose, rather unstable, and they could be easily destroyed by ultrasonic treatment. Addition of Triton X-100 with concentrations up to CMC does not change the ζ-potential, but results in high aggregation stability of CNTs aqueous suspension.

6-10.P

CLUSTERIZATION ASPECTS OF FULLERENE C_{60} AND C_{70} IN TOLUENE/N-METHYL-2-PYRROLIDONE MIXTURE ACCORDING TO SANS, SAXS AND DLS DATA

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Since fullerenes were discovered potential applications of fullerene solutions in various fields including electronics, optics, cosmetics, and pharmaceutics were intensively studied [1-3]. Despite of a wide application of fullerene solutions, the processes of their aggregation are still not clear in both weakly polar solvents and their mixtures with polar solvents [4]. Having a good solubility in different nitrogen-containing solvents, the systems based on the fullerenes C60 and C70 show a high sensitivity of optical properties to the change of liquid medium, an addition of miscible solvents to them.
N-methyl-2-pyrrolidone (NMP) is a comparatively good solvent for molecules C60 and C70 and it is also mixable with water. This solvent is suitable for fullerene transferee into aqueous media that is important for employing biological functionalized fullerenes in medical applications [5, 6].
The change in the absorption UV-Vis spectrum of the systems C60/NMP and C70/NMP varying the composition of the systems by admixing water of another extra solvents is well-known as solvatochromic effect. The phenomenon could be related with the appearance of donor-acceptor complexes between C60 (C70) and solvents molecules on the cluster surface. At the same time it has a temporal character that can be connected with aggregation of fullerene monomers in the systems or their reorganization. Thus, the two effects competing determine the existence of the solvatochromic effect in C60/NMP and C70/NMP systems.
Solutions of the fullerenes C60 and C70 in polar and non-polar solvents and their mixtures are characterized by various effects, such as the unexpected aggregation in “good” fullerene solvents, or solvatochromic effects in solvent mixtures. The question under study in the present work is at what extent the solvatochromism (change in the absorption UV -Vis spectrum with time) is determined by the cluster formation in toluene (ε=2.4)-NMP(ε=32) mixture.

References

[1] L. Wang, *J. Phys. Chem. Solids*, **84,** 85-95 (2015).
[2] M. Xing, R. Wang, J. Yu, *Int. J. Refrigeration*, **40**, 398-403, (2014).
[3] S. Afreen, K. Muthoosamy, S. Manickam, U. Hashim, *Biosensors and Bioelectronics*, **63**, 354-364 (2015).
[4] T.V. Tropin, M.V. Avdeev, O.A. Kyzyma, V.L. Aksenov, *Phys. Status Solidi B*, **247** (11-12) 3022-3025 (2010).
[5] J.D. Fortner, D.Y. Lyon, C.M. Sayes, A.M. Boyd et.al, *Environ Sci Technol* **39** 4307-4316 (2005).
[6] E. Oberdorster, *Environ. Health Perspect*. **112** 1058-1062 (2004).

6-11.P

MODIFIED CARBON NANOPOWDERS FOR COMPOSITE ELECTROCHEMICAL COATINGS

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Carbon nanopowders (multilayered carbon nanotubes, diamond detonation synthesis), which are uniform in size, chemical and energy state of the surface are necessary to create stable suspensions used in the manufacture of composite electrochemical coatings. Carbon nanopowders: of multilayered carbon nanotubes, of diamond detonation synthesis, uniform in size, chemical and energy state of the surface are necessary to create stable suspensions used in the manufacture of composite electrochemical coatings.
The purpose of this work is to disassemble the method of modifying carbon nanopowders, which makes it possible to obtain powders that are uniform in size, chemical and energy state of the surface.
Based on the results of the research, the methodology and the schematic scheme for modifying powders has been developed, which consists of chemical removal of impurities of metals and their compounds, sedimentation of powder particles under dynamic conditions to produce powders of various classes of size and uniformity, and electrochemical processing.
The method provides carbon nanopowders with a reduced impurity content of 12-45%; increased uniformity in size 1.6-3.5 times; increased specific surface area by 5.6%, reduced adsorption (by 33.8%) and electrokinetic (by 48%) potentials; increased by 2.7 times chemically homogeneous surface. Stability of aqueous suspensions of such powders increases ~2.

6-12.P

PHOTOSENTISATION OF CARBON NANOSTRUCTURES WITH POLYMETHINE DYES

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The multifunctional properties of carbon nanostructures make them a basis for a lot of applications. Addition to the carbon nanostructures polymethine dyes – by covalent bonding or stacking interaction - leads to appearance of new optical properties of such systems. The latter complexes are formed through Coulomb attractions between dye molecules with uncompensated charges and carbon nanostructures. The electron structure of such systems can be modified for creation of molecules with controlled properties, for example, molecular systems for photodynamic therapy. We have studied properties of new synthesized molecule C60- pentamethinecyanine dye in comparision with the separate dye using UV-Vis, stationary and time-dependent luminescence spectroscopy and quantum-chemical calculations.

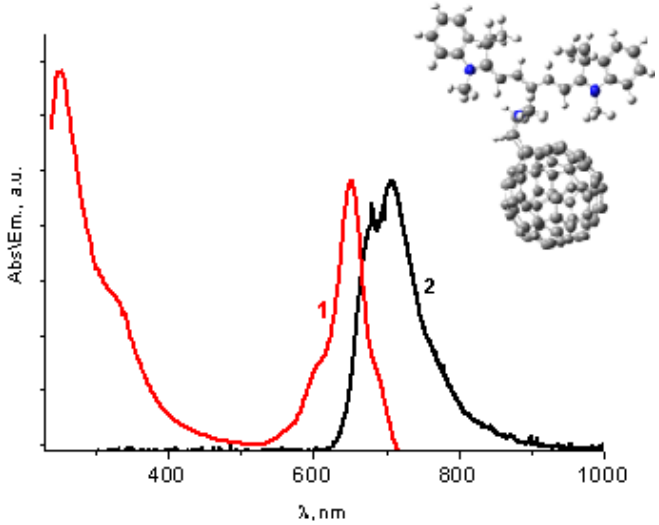

Fig. 1. Absorption (1) and luminescence (2) spectra of C60- pentamethinecyanine dye.

It was established that in the case of a covalent bond of fullerene with the dye the absorption band with maximal intensity is caused by absorption of the chromophore, while the stack interaction is characterized by absorption bands in the infrared region.

The molecule C_{60}- pentamethinecyanine dye absorbs in in so called therapeutic window and due to time of living of 2 ns in the triplet state can be applied as photo sensitizer in photodynamic therapy.

SURFACE TENSION AND SATURATED VAPOR PRESSURE OF NANOFLUIDS OF ISOPROPANOL/AL_2O_3 NANOPARTICLES AND O-XYLENE/C_{60} FULLERENES

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Information on surface tension is necessary for modeling boiling processes in nanofluids. It should be noted that the surface tension of liquids and the saturated vapor pressure are due to a specific intermolecular interaction in the region of spatial heterogeneity of the substance (surface layer). Moreover, the compositions of the surface layer of solution and its liquid phase are not equal [1]. The presence of nanoparticles in the base fluid affects the composition and structure of the surface layer of liquids. However, there are no methods for determining the composition of the surface layer of nanofluids and this fact complicates establishing the dependence of the surface tension on the state parameters of nanofluids.

It should be mentioned that the number of possible methodological errors in measurements of the saturated vapor pressure of nanofluids is significantly lower than for the surface tension measurements. Therefore, in the development of models for predicting the surface tension, scientific and practical interest has establishing the relation between the surface tension and the saturated vapor pressure of nanofluids.

In the presented work, we consider nanofluids of isopropanol/Al_2O_3 nanoparticles and o-xylene/fullerenes C_{60}. Saturated vapor pressure and surface tension of nanofluids of isopropanol/Al_2O_3 nanoparticles have been studied in the temperature range 10-70 ^{0}C and concentrations 0-9,5 wt.% of Al_2O_3 nanoparticles. Measurement of saturated vapor pressure and surface tension of nanofluids of o-xylene/fullerenes C_{60} have been performed in the temperature range 10-70 ^{0}C and the concentration range 0-0,74 wt.%. It is shown that additives of Al_2O_3 nanoparticles and fullerenes C_{60} lead to a decrease in the surface tension and increase in the saturated vapor pressure.

We present the results of the analysis of the relation between the reduced surface tension

$$\varphi(t) = \frac{\sigma(t)}{\sigma_{nb}} \qquad (1)$$

and the reduced saturated vapor pressure

$$\pi(t) = ln\left(\frac{\overline{P_c}}{P_s(t)}\right), \qquad (2)$$

where σ_{nb} is the surface tension of saturated liquid at normal boiling point; $\overline{P_c}$ is the pseudocritical pressure; $t = 1 - \frac{T}{T_c}$ is the reduced temperature; $\overline{T_c}$ is the pseudocritical temperature.

It is shown that there is a universal dependence between the reduced surface tension and saturated vapor pressure for the researched nanofluids.

References

[1] Zhelezny V., Sechenyh V., Ivchenko D., Semenyuk Yu. Prediction of the surface tension for refrigerants and refrigerant-oil solutions (ROS). *International Journal of Refrigeration*. 2014. Vol.40. P. 241 -245.

6-14.P

THE EFFECT OF FULLERENES C_{60} ADDITIVES ON DENSITY, VISCOSITY AND HEAT CAPACITY OF O-XYLENE

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The use of nanofluids in solar thermal collectors as perspective coolants to directly absorb the lights is an actively developing direction in alternative energy. The use of such collectors can increase the efficiency of production of "green" thermal energy. Information on the density, viscosity, and heat capacity of nanocoolants with direct absorption of solar energy is important both in the design of collectors and in evaluating the regime parameters of their operation.

The use of fullerenes C_{60} as a component of coolants will increase the absorption of sunlight, which will lead to an increase in the efficiency parameters of solar collectors. In a number of organic liquids, fullerenes C_{60} dissolve to molecules and only after reaching a certain concentration (depending on the solvent) begin to form clusters. Thus, at a correctly chosen concentration, the fullerenes in the solution do not aggregate and sediment with time, unlike carbon nanotubes or metal nanoparticles. This is an important technological advantage of nanocoolants based on organic liquids and fullerenes.

The purpose of this study was to evaluate the effect of fullerene additives on density, viscosity, and heat capacity of o-xylene. o-Xylene has been chosen as a model fluid because its thermophysical properties and solubility of fullerenes C_{60} in it are well studied.

The report presents data on the viscosity and density of solutions of o-xylene/fullerenes C_{60} with concentrations 0.55 and 0.74 wt.% in the temperature range of 273 – 233 K. It was shown that fullerene additives lead to a slight (up to 1.5% for C_{60} concentration of 0.55 wt.%) increase in the viscosity of o-xylene. The effect of fullerene additives (0.55 wt.%) on the density of o-xylene was insignificant (within the uncertainty of the experimental data).

The report also presents the results of a study of the effect of fullerenes C_{60} on the caloric properties of o-xylene in solid and liquid phases in the temperature range from 90 K to 340 K. The influence of fullerenes on the parameters of the solid-liquid phase transition was studied. It was shown that the additives of fullerenes C_{60} (0.55 wt.%) lead to a decrease in the heat of the phase transition and practically do not affect the melting point of o-xylene. The presence of fullerene additives in o-xylene leads to an insignificant increase in the heat capacity in the solid and liquid phases.

SPECIFIC FEATURES OF FULLERENES IN BINARY MIXTURES: NEW OPPORTUNITIES FOR BIOMEDICINE

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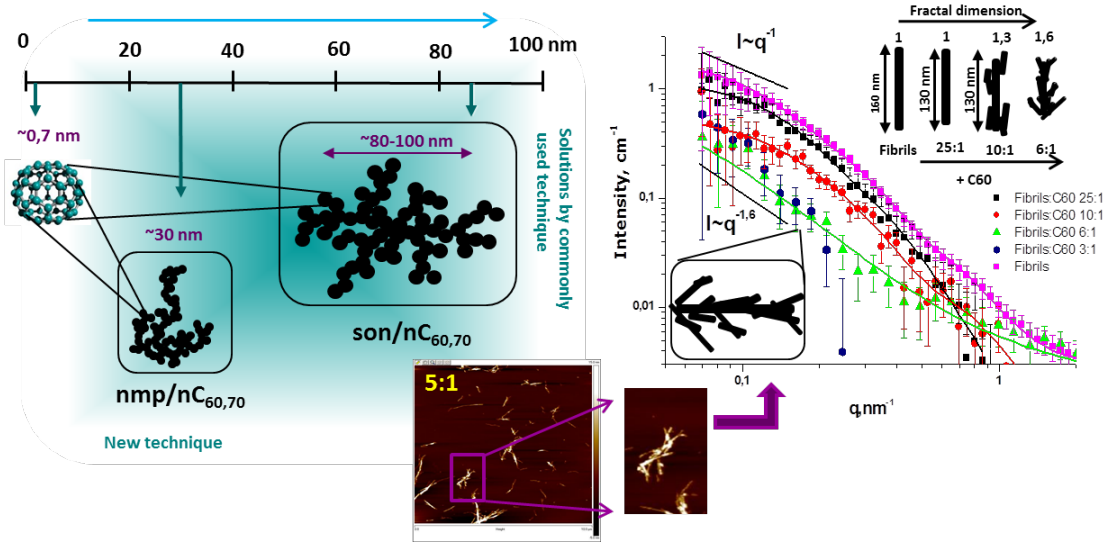
The increase in the applications of fullerenes in various fields including electronics, optics, cosmetics, and pharmaceutics raises the requirements for control of dimensions of the fullerene aggregates in various solvents. First of all, this concerns solutions in polar solvents and their mixtures, due to low fullerene solubility in them. Dissolution and equilibration of fullerenes in solvents is a complex kinetic process accompanied by various effects, such as the unexpected aggregation in solvents with good fullerene solubility or solvatochromic shifts in absorption spectra [1,2]. Despite numerous papers devoted to fullerene dispersions the behavior of fullerenes is still unclear upon transition from an organic solvent to a polar environment [3].

The work concerns the problem of aggregation of fullerenes in various systems and accompanying effects. The changes in the UV-Vis spectra observed when varying the solvent mixture composition are discussed. The interesting fact discovered is that solvatochromism as well as the cluster size of fullerenes strongly depend on the order of the mixture preparation. As a result, a new method of fullerene dissolution in water was suggested. The obtained aqueous solution of fullerenes C_{60} and C_{70} are characterized by the small size of the fullerene aggregates, in comparison with the solutions synthesized by the previously known techniques. The new solutions show a low toxicity and, according to SANS data, effectively destroyed amyloid fibrils, which responsible for neurodegenerative Alzheimer's and Parkinson's diseases.



References

[1] O.A. Kyzyma, T.O. Kyrey, M.V. Avdeev, et al. Chem. Phys. Lett. 556 (2013) 178.
Nagorna T.V., Kyzyma O.A., Chudoba D., et al. J. Mol. Liq. 235(2017)111.
[2] N. O. Mchedlov-Petrossyan, Chem. Rev. 113 (7) (2013) 5149.

Section 7. Colloidal Systems: Nano-Diamonds, Magnetic Particles and Laponite Suspensions

Oral session

7-1.O

FERRONEMATICS- LIQUID CRYSTALLINE SENSORS OF MAGNETIC FIELDS

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Liquid crystals (LCs) respond very sensitively to external electric field, whereas they are weakly sensitive to magnetic field. A possible way to improving that sensitivity is doping LCs with magnetic nanoparticles (MNPs). As a result, stable colloidal suspensions of LCs with relatively low concentrations of MNPs, called ferronematics (FNs), can be produced. These suspensions are considered to be extremely promising materials that may serve as sensor of small magnetic fields.

In the presentation will be illustrated experimental data regarding the effect of shape and size of used MNPs in thermotropic and lyotropic LCs [1], response of these systems in low magnetic field region [2]. Behavior of these systems opens the doors towards their application such as low magnetic field sensors [3] or basic logical elements for information storage technologies. A new method of detecting low magnetic fields by Whispering gallery mode (WGM) will be also presented. The experimental results demonstrated that the proposed sensor was more sensitive for samples of LC infiltrated with MNPs than for undoped LC [4]. This is the way to obtain magnetovision camera with the possibility of mapping the magnetic field in space.

References

[1] P. Kopcansky et al., *Phys. Rev. E* **78**, 011702 (2008).
[2] N. Tomasovicova et al., *Phys. Rev. E* **87**, 01450 (2013).
[3] N. Tomasovicova et al., *Soft Matter* **12**, 5780 (2016).
[4] A. Mahmood et al., *Optics Express* **25**, 12195 (2017).

STUDY OF GROWTH OF THE TETRAETHOXYSILANE CLUSTERS IN BASIC ETHANOL/WATER SOLUTIONS: SANS CONTRAST VARIATION STUDY

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The study of the structure of branched polymeric materials is of current interest because of its great role in modern technologies. The classical material most widely used to produce silicon-based branched polymers is silicon tetraethoxide (TEOS) [1-2]. After hydrolysis in alcohol-water solutions it forms clusters, which results in a wide class of different structures [3-5] depending on the number of parameters like pH, H2O/TEOS molar ratio, total TEOS concentration etc.

In present research small-angle neutron scattering (SANS) with the inner and outer contrast variation (H/D substitution) was applied to aggregates in hydrolyzed solutions of TEOS in ethanol. The task was to find out characteristics of the distribution of the scattering length density inside the clusters and conclude how much hydroxyl and ethyl groups are included in the final aggregate structure (both bulk and surface), as well as how far this depends on the conditions of the synthesis.

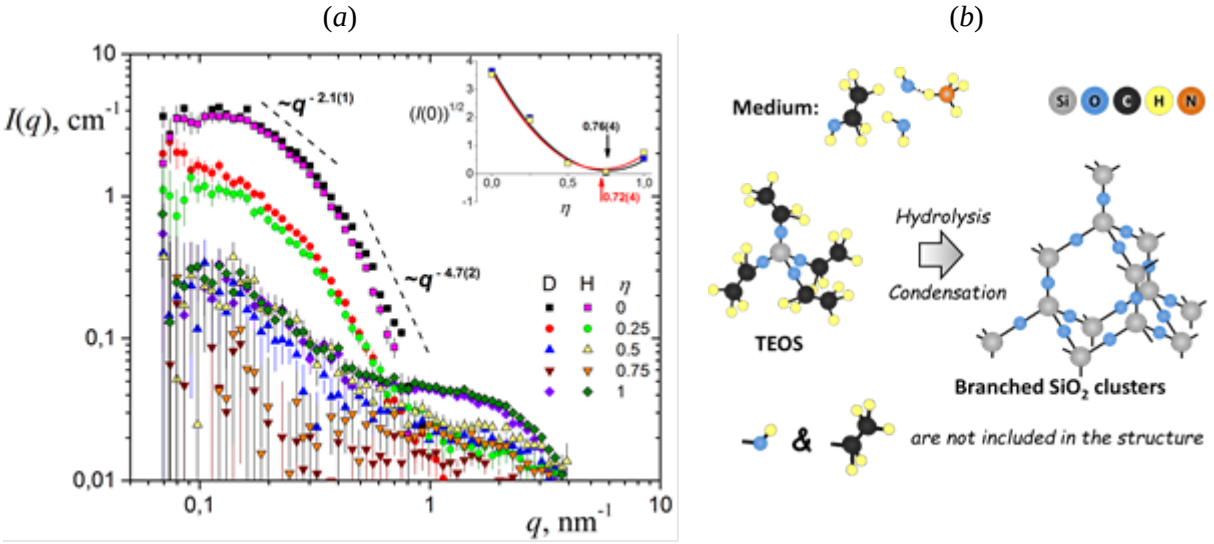

Fig. 1. (*a*) Contrast variation in SANS from two types of the studied systems, based on light and heavy water. Inset shows experimentally obtained values of square roots of forward scattering intensities as functions of the d-ethanol volume content (η) together with corresponding parabolic approximations and match-points. (*b*) Molecular models of the components of the initial solution and resulting silica clusters.

Obtained data indicate that the structure of clusters does not contain closed hydroxyl groups. Thus, the overwhelming majority of the hydrolyzed bonds participate in the condensation reaction to form Si-O-Si structure units. The temporal dependence of cluster growth was investigated together with the dependence of the structure of a liquid nanosystem under study on the parameters of synthesis.

References

[1] R.K. Iler, The chemistry of silica: solubility, polymerization, colloid and surface properties, and biochemistry, New York: Wiley, 866 p. (1979).
[2] L. Rösch, P. John, R. Reitmeier. Silicon compounds, organic. In: Ullmann's Encyclopedia of Industrial Chemistry, Weinheim: Wiley-VCH, P.637-674. (2000).
[3] D.W. Schaefer, K.D. Keefer, *Phys. Rev. Lett.* **53**, 1383-1386 (1984).
[4] K.D. Keefer, D.W. Schaefer, *Phys. Rev. Lett.* **56**, 2376-2379 (1986).
[5] M.V. Avdeev, V.L. Aksenov, J. Kohlbrecher, L. Rosta, *Physica B* **350**, e905-e908 (2004).

KINETICS OF INTERACTION BETWEEN DOXORUBICIN AND MAGNETITE NANOPARTICLES

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An anthracycline antibiotic doxorubicin hydrochloride (DOX) is a highly effective drug used in the chemotherapy of a variety of cancers [1]. The side effects of DOX such as cardiotoxicity can be diminished by direct targeting of the drug to the tumor using magnetic nanoparticles and its subsequent retention there under the external magnetic field. The potential practical application of the drug depends on its adsorption and desorption processes. In the present work, we investigated the kinetics of adsorption of DOX molecules on the magnetite nanoparticles (MNP) coated with sodium citrate and desorption of the drug from their surface.

Suspensions containing MNP prepared in trisodium citrate and DOX were processed by ultrasound dispersion. The colloid solutions were placed on the samarium-cobalt magnet for 10 minutes in order for nanoparticles with a bound drug to precipitate. We consider the supernatant to contain only a free drug. Its spectra were recorded in the visible spectrum region.

In order to determine the efficiency of MNP as drug carriers, the kinetic curve of adsorption of DOX molecules on MNP surface was constructed. According to the kinetic studies, more than 65% of DOX molecules get loaded on the nanoparticles in the first three hours.

For the desorption experiment, the supernatant was removed from the suspensions and the equal volume of distilled water was added to the sorbent residue. In the obtained solutions, the released drug concentration in the supernatant was determined from its adsorption spectra at given time intervals.

Our results show that desorption process is very slow: after more than 28 hours only about 10% of adsorbed DOX.

We show that none of the commonly used kinetic models of adsorption (pseudo-first and pseudo-second order) describe the experimental kinetics data.

References

[1] H. K. Al-Hakeim, M. M. Redha, A. H. Dawood. *Der Chemica Sinica*, **6(5)**, 137-146 (2015).

MANGANITE NANOPARTICLES OF $La_{1-x}Sr_xMnO_3$ AND MAGNETIC FLUIDS BASED ON THEM

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$La_{1-x}Sr_xMnO_3$ manganites has a Curie temperature, which depends on the chemical composition and varies in the range of 20 – 90°C [1]. Therefore, manganite nanoparticles (NPs) are promising for application in magnetic hyperthermia (local heating oncological tumors to 43 -45 C under the action of alternating magnetic field (AMF)). However, such NPs need to satisfy important requirements: weak agglomeration, small sizes, superparamagnetic properties and high heating efficiency under AC magnetic field to 43 -45 C (high specific loss power SLP).

The aim of this study is synthesis of weakly agglomerated $La_{1-x}Sr_xMnO_3$ NPs via various methods: precipitation from non-aqueous solution, from microemulsion, sol-gel method, preparation of magnetic fluids and studying their heating efficiency in AMF.

As the result of performed studies, it has been shown that independently on the method an amorphous powder has been obtained after synthesis. Crystalline $La_{1-x}Sr_xMnO_3$ NPs has been formed at 600 – 800°C in one-stage that leads to particles agglomeration. It has been established that particles have different size and heating efficiency in AMF dependently on the method of synthesis (Table).

Table. Parameters of $La_{1-x}Sr_xMnO_3$ NPs synthesized via different methods

Method of synthesis of $La_{1-x}Sr_xMnO_3$	**Sol-gel**	**Precipitation from non-aqueous (DEG) solution**	**Synthesis from microemulsion based on CTAB**
d (nm)	30 – 40	20 – 30	20 – 35
SLP (W/g)	37	15	21

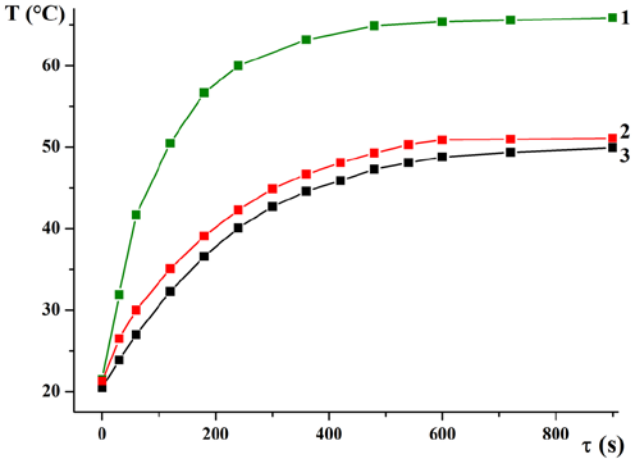

Figure. Dependences of heating temperature vs time for $La_{1-x}Sr_xMnO_3$ NPs synthesized via sol-gel method (1), precipitation from microemulsion (2) and precipitation from non-aqueous solution (3)

It has been shown that heating efficiency of NPs in AMF significantly depends on the particles size, and NPs of $La_{1-x}Sr_xMnO_3$, synthesized via sol-gel method has demonstrated better characteristic. Taking into account the requirements to magnetic NPs, one can conclude that such particles are more suitable as promising inducers in magnetic hyperthermia treatment.

References

[1] A. Urushibara, Y. Moritomo et al. *Phys. Rev. B*, **51**, 14103 – 14109 (1995).

OPTICAL EXTINCTION MEASUREMENTS USING FOR CLUSTER STRUCTURE CONTROL IN FERROFLUID LAYERS

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The new century ferrofluid (FF) topicality revival is related to new application trends: local tumor hyperthermia [1], magnetic targeted in vivo drug delivery [2] and others [3]. The FF properties (magnetic permeability tensor, saturation magnetization, viscosity, and other properties) could be varied by its integral parts changes, for instance, in the carrier liquid and the type and concentration of nanoparticles. However, even without modification of such components, the FF properties could vary via magnetic nanoparticle aggregation phenomenon.

It has been shown that timestamp of a minimal optical extinction corresponds to columnar aggregates diameter in the order of magnitude of a laser wavelength [4]. The main aim of the present work was to study the corresponding spectral dependence. The observations may reveal a quantitative information about the FF submicron structure that can be used, particularly, for preparation of composite materials.

The variations of optical transmission extinction value in a magnetic field have been described using the relative optical transmission coefficient $T = I_1/I_2$, where I_2 (I_1) is an optical radiation intensity that passed the FF sample before (after) turning on the magnetic field pulse. It was shown [4] that long-term magnetic field pulse application to FF layers leads to an emergence of an optical extinction trend inversion (OETI) phenomenon, which could be described in details as follows. The FF transparency decreases after the magnetic field pulse rising edge (timestamp τ_0) for the time interval τ_1. Then, the FF transparency starts growing until the magnetic field falling edge τ_o (Fig. 1a) followed by a recovery of the initial optical transmission.

The OETI phenomenon was investigated at four different wavelengths (λ_B=450 ± 10 nm, λ_G=530 ± 10 nm, λ_R=630 nm, λ_{IR}=1060 ± 10 nm) and different magnetic field magnitudes.

References

[1] A. Jordan, R. Scholz, P. Wust and H. Fähling, J. Magn. Magn. Mater., **201,** P. 413–419 (1999).
[2] A.S. Lübbe, C. Alexiou and C. Bergemann, J. Surg. Res., **95**, P. 200–206 (2001).
[4] S.I. Shulyma, B.M. Tanygin, V.F. Kovalenko and M.V. Petrychuk, J. Magn. Magn. Mater., **416,** P. 141–149 (2016).

IMPACT OF POLY (ETHYLENE GLYCOL) ADDITION ON THE STRUCTURE AND INTERACTION PARAMETERS OF ANIONIC SURFACTANT MICELLAR SOLUTION

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Micellar systems of surfactants play important role in production of stable colloidal solutions in various applications. Thus, for water solutions of anionic surfactants sodium oleate (SO) and dodecylbenzene sulphonic asid (DBSA) used for double layer sterical stabilization of magnetic nanoparticles in aqueous ferrofluids the physicochemical properties of micelles have influence on the structural organization ferrofluids [1]. The properties of ferrofluids can be modified by adding polymers into their structure. In this respect, the resulting multicomponent system with micelle-polymer buffer tends to the aggregate structure reorganization [2]. The present work is dedicated to the investigations of structural and interaction parameters of SO and DBSA micellar systems under effect of addition of water-soluble neutral polymer poly (ethylene glycol) (PEG). This polymer is used, in particular, in practice to improve biocompatibility of ferrofluids. Small-angle neutron scattering (SANS) together with the surface tension study allowed us to determine a number of micelle parameters including the aggregation number, degree of ionization, axial ratio of micelle shape and inverse screening length for various compositions of the mixed solutions. The presence of polymer-micelle interaction and polymer-surfactant complex formation in the range of characteristic concentration from critical aggregation concentration (CAC) to critical micelle aggregation (CMC) was observed by the tensiometric technique. The formation of micelles with morphology close to spherical (no transition to prolong ellipsoids), large degree of ionization (up to 25%) and larger value of reverse screening length as compared to free surfactant solutions were found from the analysis of the concentration dependences of the mentioned above parameters for different surfactant/polymer ratios and for different molecular mass of PEG (1- 20 kDa). A similar screening effect for SO-PEG 1 kDa systems was observed in our previous work [3]

References

[1] Petrenko V. I., Artykulnyi O. P., Bulavin L. A., Almásy L., Garamus V. M., Ivankov O. I., Avdeev, M. V, *Coll. Surf. A.* (2017).
[2] Avdeev M. V., Feoktystov A. V., Kopcansky P., Lancz G., Garamus V. M., Willumeit R., Jurikova A., *J. Appl. Cryst.* **43(5)**, 959-969 (2010).
[3] Petrenko V. I., Avdeev M. V., Garamus V. M., Bulavin L. A., Kopcansky P., *Coll. Surf. A.* **480**, 191-196 (2015).

ELECTROPHORESIS OF HIGHLY ANISOMETRIC PARTICLES IN AQUEOUS SUSPENSIONS: WEAK AND STRONG ELECTRIC FIELDS

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The electric response of highly anisometric particles (carbon nanotubes, fibers, viruses, clay mineral platelets, biological macromolecules, etc.) to the applied field, *E*, continuously attracts commercial and academic interest. The electrophoretic mobility, *U*, of anisometric particles can depend on their orientation in the electric field. For example, it has demonstrated (Henry) that
(i) the classical Smoluchowski equation (the relationship between electrophoretic velocity, V_{ef}, electric field strength, *E*, and solution characteristics) holds for particles of any shape provided that the thickness of the electrical double layer (EDL) is much smaller than the shortest characteristic length of the particle, and
(ii) The effect of the ionic strength on the mobility of long cylindrical particles depends on their orientation, and it is unessential for particles aligned along the applied field, and important for perpendicular orientation with respect to *E*. The modification can be embodied in a correcting factor, ranging from 1/2 to 1, as the ionic strength changes from low to high.
The Henry model was later modified for the soft cylindrical particles (Oshima), or considering the effect of the EDL polarization (Dukhin) on the electrophoresis at parallel and perpendicular orientation of particles in the electric field.
This work summarizes the recent studies on electrophoresis of multi-walled carbon nanotubes (diameter of 10-20 nm and length of 5-10 μm, CNT), inorganic nano-platelets (synthetic Laponite® RD, diameter of ≈25 nm and width of ≈1 nm, Lap) and their hybrids in aqueous suspensions at different pH and in presence of added electrolytes (mono-, bi-and trivalent counter-ions) as well as anionic and cationic surfactants. For CNTs, an increase of pH and adsorption of anionic surfactant gives a rise to the absolute (negative) value of the zeta-potential due to increasing dissociation of the weak surface acidic functional groups or adsorption of the surfactant anion. The behavior of CNT and CNT + Lap hybrid nano-particles in ***weak electric fields*** (5-15 V/cm) corresponds to that of lyophobic colloids. Particularly, the *ζ(C)* plots for 1-1 electrolyte reveals a maximum, addition of 2-1 electrolyte gives a considerable decrease of the zeta-potential, whereas increasing amounts of trivalent counter-ions or cationic surfactant results in the change of the sign of nanotubes charge. Addition of Lap platelets in the range from X=0 to 0.4 (where X is the mass ratio of Lap/CNTs) causes a monotonic decrease of the ζ-potential of the CNTs So, the strong dependence of the electrophoretic mobility of CNT and CNT+Lap hybrid on the electrolyte/surfactant type and concentration is in line with the developed concept of electrophoresis of cylindrical particles.
The behaviour of unipolar conducting particles/fibres is dramatically changes ***in strong electric fields*** (several hundred V/cm). The electrophoresis in this case is arisen due to the interaction of a strong outer field with a secondary diffuse layer of counter-ions (space charge). This layer is induced outside the primary (classical) diffuse EDL by the external field itself because of concentration polarization. For spherical conducting particles the theory (Dukhin-Mishchuk) predicts linear dependence of the electrophoretic velocity on the particle's size and superfast quadratic dependence on the external electric field strength, $V_{ef} \sim E^2$. A method to determine the huge electrophoretic velocities (mm/sec or cm/sec) in strong fields has been developed. The electrophoretic velocity, V_{ef}, of ion-type conducting polyacrylonitrile ion-exchanger fibers and (for sake of comparison) non-conducting polyphenylenisophtalamide fibers as a function of their length and the electric field strength (2-500 V/cm) was studied. The superfast electrophoresis with quadratic dependence $V_{ef} \sim E^2$ was observed for conducting fibers and the observed trends for anisometric particles were quantitatively similar to those for spherical particles.

This study was in part supported by the Program (GINOP-2.3.4-15-2016-00004), the National Academy of Sciences of Ukraine, Project No. 43/18-H and and the cooperation agreement between Hungarian and Ukrainian Academies of Sciences.

LOCUS AND LOCAL ENVIRONMENT OF TWO DYES IN SURFACTANT MICELLES FROM MOLECULAR DYNAMICS SIMULATIONS

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One of the most important properties of a colloid particle is its surface electrical potential, Ψ, which ultimately determines the effect of the particles on the adsorbed compounds. For surfactant micelles, the values of Ψ are usually derived from experimental measurements of acidity constants of dyes adsorbed at them via Eq. 1 [1,2].

$$\mathrm{p}K_\mathrm{a}^\mathrm{app} = \mathrm{p}K_\mathrm{a}^\mathrm{w} + \log\frac{{}^\mathrm{w}\gamma_{\mathrm{D}^-}^\mathrm{m}}{{}^\mathrm{w}\gamma_\mathrm{HD}^\mathrm{m}} - \frac{\Psi F}{RT\ln 10} \quad (1)$$

However, the calculation requires some assumptions about the second term of the rhs to be made. Their correctness relies on the estimates of the local environments of the neutral and charged forms of the dye molecule. Therefore, in order to validate them, we performed all-atom molecular dynamics simulations of two dyes, namely, diphenylazo-o-nitrophenol (DNP) and 4-n-heptadecyl-7-hydroxycoumarin (HHC), in cationic (CTAB, CPC) and anionic (SDS, SCSn) micelles, to compare the locus and local environment of neutral and anionic forms of the dyes' molecules.

The results show that both dyes are located in the Stern layer (except for the hydrocarbon tail of HHC that is immersed into micelle core). For DNP, the orientations of two charge forms are considerably different, while for HHC, they are almost identical. However, the local environments vary significantly, and the difference is somewhat higher in anionic micelles than in cationic, Fig. 1. This allows suppose that the error of Ψ values, obtained using these dyes as indicators, is higher in anionic micelles. The local environment was quantified by calculating numbers of various atoms of the medium located in 0.4 nm vicinity of the whole molecule or its O atom.

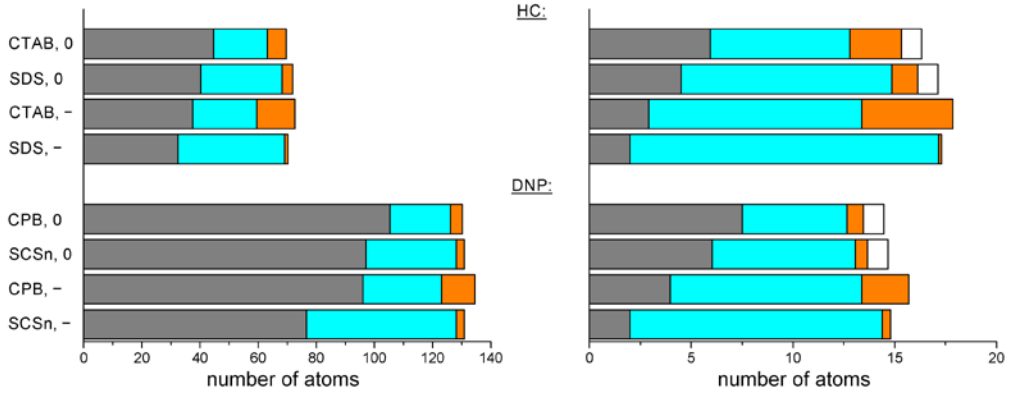

Figure 1. Compositions of local environments of HHC (top) and DNP (bottom). Left charts are for the whole molecule, right charts are for O atoms only. Sections: hydrocarbon core, water, head groups, hydroxyl H atom.

References

[1] N.O. Mchedlov-Petrossyan, *Pure Appl. Chem.*, **80**, 1459–1510 (1990).
[2] V.S. Farafonov, A.V. Lebed, N.O. Mchedlov-Petrossyan, *Colloids Surf., A.*, **538**, 583–592 (2018).

7-9.O

MOLECULAR DYNAMICS SIMULATION OF SILVER NANOPARTICLES FUNCTIONALIZED WITH STIMULI-RESPONSIVE POLYMERS

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Water-soluble polymers composed of flexible polymer chains are widely used for chemical modification of silver nanoparticles (AgNPs). Stimuli-responsive polymers, also called 'smart' polymers, can provide a promising alternative because of their capability to response to a small variation of pH, salt concentrations or temperature by making a great change in their physical characters, such as solubility and conformation. AgNPs functionalized with smart polymers can be utilized for the preparation of so-called 'smart' drug delivery systems, which mimic biological response behavior. For better understanding of the adsorption behavior of pH and temperature responsive polymers onto a silver surface, we developed their atomistic models for molecular dynamics (MD) simulation.

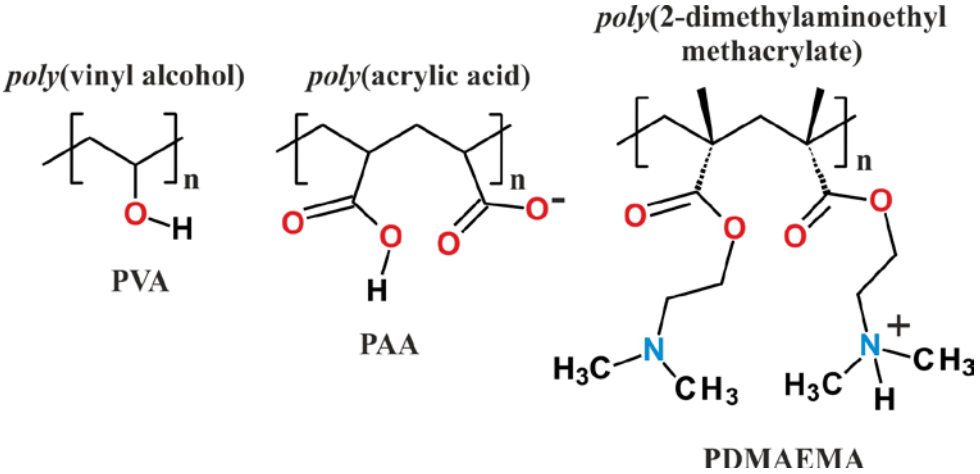

Figure 1. Structure of polymeric stabilizing agents: PVA, PAA, and PDMAEMA.

The structural features of quasi-spherical AgNPs, decorated with various organic polymers, are investigated by means of classical MD simulations as a function of a polymer chain length and a degree of protonation of their functional groups (Fig. 1). Our model approximates AgNP with a quasi-spherical silver nanocrystal with diameter 3.9 nm [1] and uses a united-atom representation for polymers [2]. Our outcomes demonstrate that the adsorption behavior of PAA and PDMAEMA depends strongly on their degree of protonation, as compared to a well-known conventional stabilizing agent PVA. Our results provide insight for the rational design of novel "smart" nanometerials and devices.

References

[1] A. Kyrychenko, O. M. Korsun, I. I. Gubin, S. M. Kovalenko, O. N. Kalugin, *J. Phys. Chem. C* **119**, 7888-7899 (2015).
[2] A. Kyrychenko, D. A. Pasko, O. N. Kalugin, *Phys. Chem. Chem. Phys.* **19**, 8742-8756 (2017).

7-10.O

DECOMPOSITION OF COLLOIDAL SUSPENSIONS OF DIELECTRIC NANOPARTICLES IN DIELECTRIC LIQUID BY EXTERNAL ELECTRIC FIELD

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Theoretical approach to describe decomposition of colloidal suspensions of dielectric nanoparticles in dielectric liquid by external electric field is developed via Poincare formalism.
Let us consider small spherical dielectric particles placed in dielectric liquid. Particles can freely diffuse through the liquid. An electric dipole moment of particles equals to zero in the absence of the external electric field. Under applied electric field the induced electric dipoles interact with external field and with each other. This leads to additional movement (together with Brownian motion) of the particles. As a result an initial homogenous distribution of particles can become non-homogenous. Indeed, the external field induces dipole moments oriented in the same way. Such dipoles are attracted. Then, if as a result of thermal fluctuations the density of particles in some place increases, other particles will be attracted to the same place as a result of this dipole interaction.
Transition to an inhomogeneous distribution has a threshold character. It occurs if the applied electric field is sufficiently strong and (or) the temperature is sufficiently low. The reason of the inhomogeneous development is polarization of the particles and their interaction as dipoles.
The critical value of the applied field increases with increasing temperature, with a decrease in the number of particles and their radius. The critical value of the applied field also increases with decreasing difference between the dielectric permittivities of particles and medium. If the permittivities are equal, the distribution of particles under the electric field remains homogeneous.
Thus, the growth of inhomogeneity should be expected for large fields, low temperatures, high particle concentration and large radius, and remarkable difference in the dielectric permittivities of particles and the medium.

7-11.O

A MANY-PARTICLE THEORY OF THE EFFECTIVE ELECTRICAL PROPERTIES OF DISPERSED SYSTEMS

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We present a self-consistent approach [1] to the effective quasistatic permittivity ε_{eff} (and, for reasons of mathematical analogy, electrical conductivity) of statistically homogeneous and isotropic dispersions of fine inhomogeneous particles. Its main points are as follows. A dispersion D to be homogenized is equivalent to an auxiliary system S prepared by embedding D's constituents (particles and matrix) into some uniform host M with unknown permittivity ε_{f}. The system S is viewed as a set of compact (small with respect to the probing field wavelength, but still macroscopic and retaining the properties of the entire S) groups of D's constituents. The permittivity distribution in S is $\varepsilon(\mathbf{r}) = \varepsilon_{\text{f}} + \delta\varepsilon(\mathbf{r})$ where $\delta\varepsilon(\mathbf{r})$ is the contribution from the local compact group. The effective electric properties of S are formed by the multiple reemissions and correlations inside such groups. The corresponding contributions to the average field and induction are extracted from the iterative series by replacing the propagators by their delta function parts. The permittivity ε_{eff} is calculated, using the compact group technique and the Hashin-Shtrikman variational theorem, through the linear constitutive equation and through the equality of the electric energies stored in S and the homogenized system. The requirement that both ways give equal results closes the equations for ε_{eff} and ε_{f}. As a result, finding ε_{eff} reduces to calculating and summing up the statistical moments of $\delta\varepsilon(\mathbf{r})$. The latter is modeled according to the suggested microstructures of D's constituents.
The efficiency of the theory is exemplified by its applications to dispersions of graded hard and hard-core–penetrable-shell particles.

References

[1] M. Ya. Sushko, *Phys. Rev. E*, **96**, 062121 (2017).

7-12.O

IS THE CLASSICAL DIFFERENTIAL SCHEME FOR PERMITTIVITY OF EMULSIONS CONSISTENT?

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The classical differential mixing rules, exemplified by the asymmetrical Bruggeman and Maxwell-Wagner-Hanai (MWH) approaches, are assumed to be independent effective-medium theories. They were originally developed for the effective permittivity ε of emulsions, for which the classical Maxwell-Garnett and Bruggeman approaches fail. Despite ignoring many important mechanisms (e.g. surface tensions of emulsion droplets), these rules are often used to process experimental data. However, while some authors believe these rules to be efficient, the others state that the basic assumptions behind them are not justified.

This report discusses the internal inconsistency and the ranges of validity of the MWH approach and its modifications. For this purpose, a generalized differential scheme is developed for ε of macroscopically homogeneous and isotropic dielectric mixtures [1]. It is based upon the compact group approach [2] reformulated so as to allow one to analyze the role of different contributions to ε. The scheme is then applied to the simplest system of impenetrable balls in a uniform medium.

It is shown that the MWH approach is recovered if the electromagnetic interaction between previously added constituents and those being added is replaced by the interaction of the latter with recursively formed effective medium. Each portion of inclusions has a different polarization, and the previously added portions do not interact with the new ones. The latter is valid only for narrow concentration ranges and low dielectric contrasts between the constituents. This conclusion remains valid for the generalizations to the MWH obtained within the developed scheme – contrary to the expectations, they even violate the Hashin-Shtrikman bounds. It follows that the MWH approach is rather approximate and must be used with caution to avoid uncontrolled errors and misinterpretation of the results.

References

[1] A. K. Semenov, *J. Phys. Commun.*, **doi: 10.1088/2399-6528/aab060** (2018).
[2] M.Ya. Sushko, *Zh. Eksp. Teor. Fiz.*, **132**, 478 (2007). [*JETP*, **105**, 426 (2007)].

7-13.O

MICROHETEROGENEOUS STRUCTURE OF OXIDE MELT

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A microheterogeneous model of the oxide melts is proposed. The base of the model is that the melt is a complex system that consists of compacted micro particles of nanometric size and a continuous disordered matrix. The matrix consists of atoms, molecules and their associates of small size. The base of the model is that the melt is a complex system that consists of compacted micro particles of nanometric size and a continuous disordered matrix [1]. The matrix consists of atoms, molecules and their associates of small size. The density of the disordered matrix is close to the gas density.

The bases of compacted nanoparticles are clusters of spherical type, where the oxygen anions form a close packing. The tetrahedral and octahedral cavities within it are occupied by metal cations. The condensed nanoparticle is in continuous diffuse interaction with the discharged matrix. The excess surface charge of the cluster is compensated by cations and anions from the discharged matrix. These particles form around the cluster alternating layers of cations and anions. The change in temperature and pressure leads to a change in the number and composition of the surface layers. With a certain long exposure at a certain temperature, equilibrium sets in.

At low temperatures (near melting), the compacted nanoparticles can self-organize into superclusters (several interconnected identical clusters). We believe that such nanoclusters are rather stable in a disordered matrix.

References

[1] A. I. Karasevskii *J. Physics: Condensed Matter*, **46**, 1-18 (2008).

INVESTIGATION OF THE VISCOSITY OF MAGNETIC FLUIDS

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It have been investigated the temperature dependence of the $FeCl_3$ magnetic fluid viscosity coefficient and the activation energy of the liquid molecule in the temperature range 0 – 80 0C.

Among the methods of preparations of magnetic fluids the chemical method is more effective. $C_{\{Ni(NO_3)_2\}_x}$

The $Ni(NO_2)_3 \cdot 6H_2O$ and $FeCl_3$ salts were dissolved in water, and this results to forming of iron and nickel zols.

Magnetic fluid $Ni(NO_2)_3 \cdot 6H_2O$ viscosity coefficient was measured using capillary viscometer. The results of the measurements are shown in figure 1.

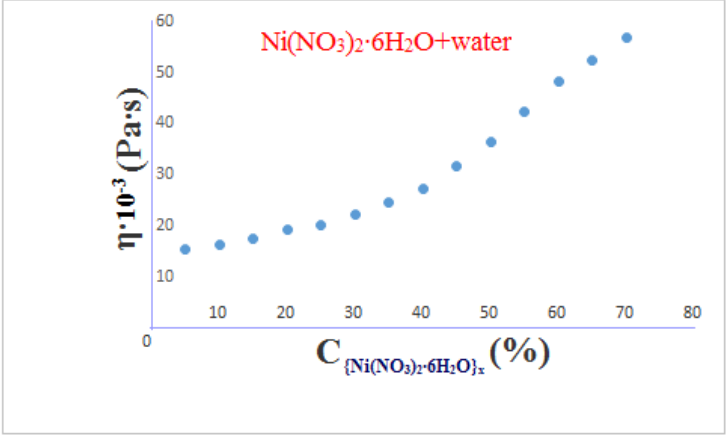

Fig.1 The dependence of magnetic fluid viscosity coefficient on concentration.

As we can see from the Fig.1 the viscosity coefficient liquid increases, with the increasing of the concentration of $Ni(NO_2)_3 \cdot 6H_2O$ solution.

The viscosity coefficient of magnetic fluids $FeCl_3$ is studied the results of the measurements are shown in Fig.2 in the temperature range 20-80 ^{0}C.

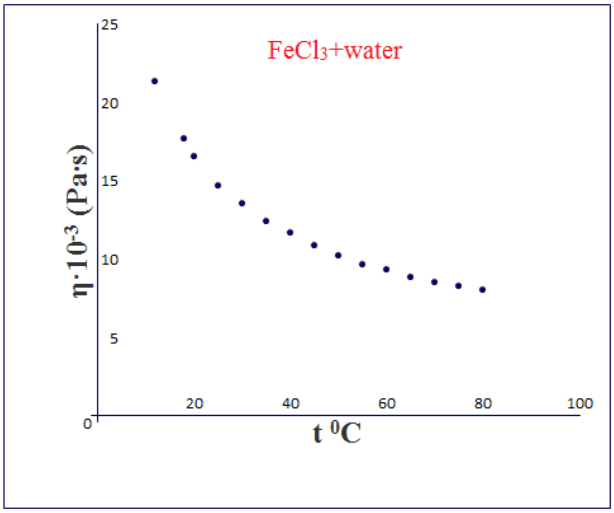

Fig.2 Temperature dependence of viscosity coefficient of the magnetic fluid.

As we can see from the Figure 2, the magnetic fluid viscosity coefficient decreases with exponential law when the temperature increases.

It is known that the temperature dependence of the viscosity coefficient of liquids can be expressed by the Frenkel-Andrade equation:

$$\eta = \eta_0 e^{\frac{E_A}{RT}} \quad (1)$$

Here, EA – is the activation energy, η0 – is the constant, k- is the Boltzmann constant, T-is the absolute temperature.
From equation (1) we can get:

$$ln\eta = ln\eta_0 + \frac{E_A}{RT} \quad (2)$$

Using the picture of dependence $\ln\eta$ from $\frac{1}{T}$ we can find the activation energy of the liquid molecule:

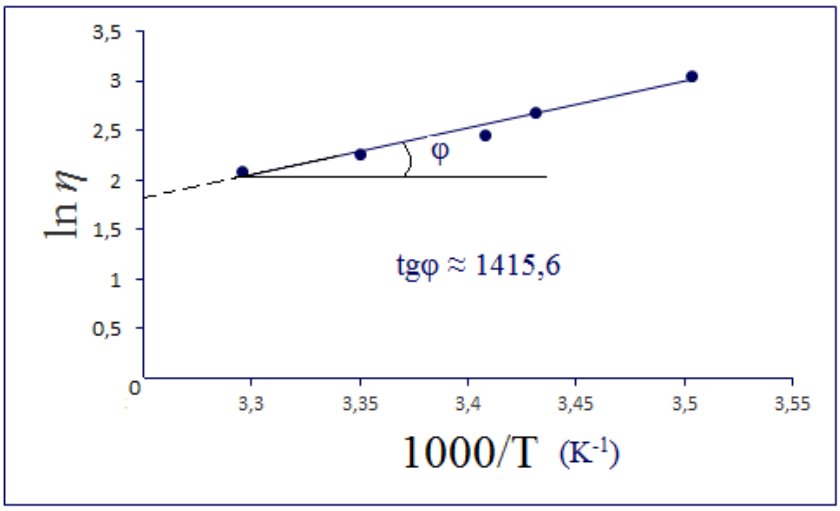

Fig.3 Dependence $\ln\eta$ from $\frac{1}{T}$

$$tg\varphi = \frac{E_A}{R}$$

$$\boldsymbol{E_A = tg\varphi \cdot R = 1415,6 \cdot 8,31 = 11,7\ \frac{kJ}{mol}}$$

HYSTERESIS OF PHYSICAL PROPERTIES OF THIXOTROPIC LIQUID INKING SYSTEM IN A PRINTING MACHINE OF ROLE AND INTAGLIO PRINTING METHODS

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The complete rheological curves of the first and second species were obtained and analyzed, depending on the magnitude of the shear stress and temperature of the base polygraphic inks of the offset role and intaglio printing methods in the temperature range (20-60)°C of their technological resistance.

The experimental results were obtained on a high-precision computerized research system on the basis of the RotoVisco1 reoviscosimeter, a measuring thermostatic liquid-type cell with a cone-plate measuring spindle by the means of constant strain rate gradient method. The cone - plate angle was 1°. The accuracy of maintaining the temperature of the test samples was ±0,01°C.

Based on the analysis of the complete rheological curves of the flow of the first and second kinds of inhomogeneous and pre-carefully homogenized paints, their main micro- and macroscopic characteristics were calculated.

It has been established that both micro- and macroscopic characteristics of non-homogenized and thoroughly homogenized paints differ in several times. So, the hysteresis of all properties of these systems is clearly manifested due to the destruction of the original structure of the paint during its homogenization. The values of the equilibrium shear modulus of the paints as a function of temperature and shear stress are given.

It is found that its value decreases by a nonlinear dependence, similar to the curve of the normal distribution law, depending on the shear stress and temperature for both non-homogenized and homogenized paints. At that, the majority of the microscopic and macroscopic parameters of non-homogenized and homogenized systems become very close in magnitude at a temperature equal to or slightly greater than 60°C, and the values of the equilibrium shear modulus at the boundary of the conditioned elasticity of the paints and the complete destruction of the initial structure begin to practically coincide at temperatures (40 ÷ 45)°C. This determines the choice of the operating temperature of the paint in the printing section of the machines during the production of the print run.

7-1.P

PLANAR ROTOR MODEL FOR DRIFT OF MAGNETIC NANOPARTICLES SUSPENDED IN A FLUID

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Recently [1,2], we have developed a deterministic theory of drift of ferromagnetic nanoparticles suspended in a fluid, which is induced by the Magnus force. Here, we present a statistical theory of this phenomenon that accounts for the influence of the rotational Brownian motion of nanoparticles on their drift velocity. Assuming that the magnetization vector is frozen into the particle body and the translational and rotational Reynolds numbers are small, we have shown [3] that the dimensionless drift velocity in the planar rotor model is given by

$$v_{\rm dr} = \int_0^1 \langle \sin\chi_{\rm st}(\xi)\rangle \sin(2\pi\xi - \phi)\, d\xi \,. \qquad (1)$$

Here, $\chi_{\rm st}(\xi) = \lim_{n\to\infty} \chi(n+\xi)$ is the lag angle between the magnetization and magnetic field in the steady state (when the dimensionless time τ equals $n+\xi$ with $n \to \infty$), ϕ is the initial phase of the periodic external force, and the angular brackets denote averaging over thermal fluctuations. The lag angle $\chi(\tau)$ satisfies the stochastic equation

$$\dot{\chi}(\tau) = \dot{\psi}(\tau) - \alpha \sin\chi(\tau) - \sqrt{2}\,\beta\,\zeta(\tau)\,, \qquad (2)$$

where the overdot denotes the derivative with respect to τ, the dimensionless parameters α and β can be associated with the inverse rotational relaxation time of nanoparticles and intensity of thermal fluctuations, respectively, $\psi(\tau)$ is the azimuthal angle of the magnetic field, which is a periodic function of τ, and $\zeta(\tau)$ is a Gaussian white noise of unit intensity. The corresponding Fokker-Planck equation for the probability density $P(\chi,\tau)$ that $\chi(\tau) =$ reads

$$\frac{\partial}{\partial\tau} P(\chi,\tau) + \dot{\psi}(\tau)\frac{\partial}{\partial\chi} P(\chi,\tau) = \alpha\frac{\partial}{\partial\chi}\sin\chi\, P(\chi,\tau) + \beta^2 \frac{\partial^2}{\partial\chi^2} P(\chi,\tau)\,. \qquad (3)$$

In the case of large thermal fluctuations, when the condition $\epsilon = \alpha/\beta^2 \ll 1$ holds, its steady-state solution $P_{\rm st}(\chi,\xi) = \lim_{n\to\infty} P(\chi, n+\xi)$ is written in the second-order approximation as

$$P_{\rm st}(\chi,\xi) = \frac{1}{2\pi} + \frac{\epsilon}{2\pi}\cos\chi + \frac{\epsilon^2}{8\pi}\cos 2\chi + \frac{\epsilon^2}{2\pi\alpha}\dot{\psi}(\xi)\sin\chi\,. \qquad (4)$$

Taking into account that $\langle \sin\chi_{\rm st}(\xi)\rangle = \int_0^{2\pi} \sin\chi\, P_{\rm st}\, d\xi$, from (1) and (4) one obtains

$$v_{\rm dr} = \frac{\epsilon^2}{2\alpha}\int_0^1 \dot{\psi}(\xi)\sin(2\pi\xi - \phi)\, d\xi\,. \qquad (5)$$

In particular, if $\psi(\tau) = \psi_m \cos(2\pi\tau)$, then (5) yields $v_{\rm dr} = -\left(\pi\psi_m\epsilon^2/2\alpha\right)\cos\phi$. We have also analytically derived the drift velocity of nanoparticles in the case of small thermal fluctuations, when $\epsilon \gg 1$.

References

[1] S.I. Denisov and B.O. Pedchenko, J. Appl. Phys., 121, 043912 (2017).
[2] S.I. Denisov, B.O. Pedchenko, O.V. Kvasnina, and E.S. Denisova, J. Magn. Magn. Mater., 443, 89 (2017).
[3] S.I. Denisov, T.V. Lyutyy, V.V. Reva, and A.S. Yermolenko, arXiv: 1711.05338.

7-2.P

STRUCTURAL-RHEOLOGICAL CHARACTERISTICS OF ISOTROPIC AND STRONGLYPOLAR LIQUIDS IN A WIDE RANGE OF TEMPERATURES OF "LIQUID-STEAM" COEXISTENCE

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Results of measurements of the viscosity of the following simple liquids have been analyzed based on the results of the authors' own researches, the research of another authors and reliable data of reference and encyclopedic editions:
1) Liquefied inert gases He, Ne, Ar, Kr, Xe;
2) Liquid nitrogen, oxygen and other gases;
3) Series of liquefied organic compounds: methane, ethane, propane, butane;
4) Liquid atomic metals with filled and unfilled outer electronic shells;
5) Molten salts: with spherical anions and cations; with nonspherical polyatomic anions;
6) Water and monohydric alcohols;
7) Some aqueous solutions of 1-1, 2-1, 3-1 electrolytes in a wide range of their concentrations and temperatures (0-100)°C.

To determine the nature of the structural changes in these systems as a function of temperature, we have introduced the notion of the degree of thermal destruction of their original structure; the numerical value of this characteristic is determined by the formula: $X_\varphi = \frac{\varphi(T)-\varphi_0}{\varphi_m-\varphi_0}$,where φ(T) is fluid mobility at a given temperature; φ_m is the mobility of the substance at the point with the minimum viscosity (at the boiling point); φ_0 - fluid mobility at a point that is close to the point of freezing (hardening) of a given fluid at a given external pressure. The admeasurement φ is defined as the ratio ρ(T)/η(T), where ρ(T) is the density of matter at a given temperature; η(T) - the admeasurement of the dynamic viscosity of the substance at a given temperature.

It is established that the course of the temperature dependence of any substance is non-linear and can be divided into a number of rectilinear sections, between the edges of which the dependence can be linear. The minimum of each interval determines the equilibrium point between the previously existing equilibrium structure of the liquid system and the subsequent (newly arising) one. The beginning and end of the linear sections determine the characteristic points (temperatures) of the liquid structures.

Highly structured fluids have concave X(T) dependences, which indicates the existence of strong collective interactions in them, associated with the thermal motion of particles; at the same time, liquid systems with spherically symmetric particles have a convex form of the X(T) dependence, which indicates the predominance in them of the individualized form of the motion of their particles. When temperature of any liquids approaches to the critical point, the degree of temperature destruction of the structure of liquid systems tends to unity over a convex curvilinear dependence.

7-3.P

MATHEMATICAL MODELING OF THE DEPENDENCE OF THE RHEOLOGICAL PROPERTIES OF LUBRICANTS AND PRINTING PAINTS OF THE ROLE OFFSET AND INTAGLIO PRINTING METHODS ON THE MAGNITUDE OF THE SHEAR STRESS AND TEMPERATURE

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Approximate analytical expressions were found for the obtained experimental dependences of rheological curves of technical lubricants similar in their component composition to printing paints, polygraphic paints of offset role and intaglio printing methods, which allow to calculate the following values depending on the shear stress and temperature: 1) the complete rheological curve of the first and second species; 2) the degree of destruction of the viscous and elastic properties of the thixotropic liquid structure; 3) equilibrium shear moduli; 4) the values of the times of Maxwellian relaxation; 5) the activation energy of viscous flow at the boundaries of: a) the conditional elasticity of the substance (with the maximum viscosity of the liquid); b) isotropic (homogeneous) state (with a minimum constant viscosity of the liquid).

The established dependencies are nonlinear, rather complex, have no analogues in the well-known printed publications and will be presented in separate publications.

STRUCTURE OF MAGNETIC FLUIDS AT INTERFACE WITH SILICON BY NEUTRON REFLECTOMETRY

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Ferrofluid(FF) is the colloidal system of magnetic nanoparticles with solvents of different polarity. Layers of surfactants are frequently used to stabilize such systems. Great interest in these systems is related due to the possibility of their use for controlled drug delivery, diagnosis and treatment of various diseases, for example cancer. Therefore, the study of biocompatible FF are very relevant. At the same time behavior of magnetic nanoparticles in the bulk and at interfaces can be very different due to specific adsorption properties, which should be considered in a variety of applications. It also remains an open question regarding the possible differences in the stability of magnetic fluids in bulk and at interfaces.

The main aim of this study is to get values of structural parameters of biocompatible ferrofluids, the study of their stability in the volume and near the surface. Information about the structure of FF in bulk was obtained from small-angle neutron scattering experiments. Neutron reflectometry experiments were done to investigate behavior of magnetic fluids with different methods of preparation and concentration at the interface with silicon. Influence of gravity on the adsorption properties of magnetic particles was also checked. It was shown that only single magnetic nanoparticles, coated by surfactant molecules, are adsorbed to the surface of the silicon from bulk of ferrofluids. X-ray reflectometry make possible to study free liquid surfaces or interfaces air/FF. It is reported about structural organization nanoparticles at this interface. Influence magnetic field with horizontal and vertical to surface direction was shown. Comparative analyses is held for all interfaces of study and volume.

A MONTE CARLO MODEL OF LIGHT PROPAGATION IN ORIENTED MEDIA FILLED BY ANISOMETRIC PARTICLES

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The Beer–Lambert–Bouguer (BLB) absorption law is widely used for description of a light propagation through composite systems filled by micro-sized and nano-sized fillers. The BLB law can be applied for highly absorbing particles, relatively small concentrations and in absence of any spatial or orientation correlations between particles. The different examples of violations of the BLB law in spatially correlated media [1] and liquid crystalline media filled with anisometric particles (carbon nanotubes and inorganic platelets) [2–5] have been already reported.

In this work the Monte Carlo method was applied to study an optical density behavior in oriented films filled by of anisometric particles. The particle shape was characterized by an aspect ratio (ratio of length l and diameter d of particle, r=h/d) and it was r>>1 for long tubes and r<<1 for thin disks. The anisotropy of distribution was characterized by order parameter, s. The correlated spatial distribution were introduced using previously developed cluster growth model [6] and characterized by aggregation parameter, f. The dependences of transmission coefficient versus the film thickness and concentration of particles at different values of r, s and f are discussed. The observed behavior was in accordance with the BLB law for stochastic and low correlated media whereas the significant deviation from the BLB law was observed for the strongly correlated media. The effective absorption cross section of particles at different values of r, s and f are also estimated.

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References

[1] T.G. Mayerhöfer, H. Mutschke, J. Popp, ChemPhysChem, **17,** 1948–1955 (2016).
[2] L.N. Lisetski, S.S. Minenko, A.S. Samoilov, N.I. Lebovka, Journal of Molecular Liquids, **235,** 90–97 (2017).
[3] L.N. Lisetski, A.P. Fedoryako, A.N. Samoilov, S.S. Minenko, M.S. Soskin, N.I. Lebovka, European Physical Journal E, **37,** 1–7 (2014).
[4] L.A. Bulavin, L.N. Lisetski, S.S. Minenko, A.N. Samoilov, V. V Klepko, S.I. Bohvan, N.I. Lebovka, Journal of Molecular Liquids, doi.org/10.1016/j.molliq.2017.12.078 (2018) (In press).
[5] A.N. Samoilov, S.S. Minenko, L.N. Lisetski, M.S. Soskin, S.I. Torgova, N.I. Lebovka, Liquid Crystals, **45,** 250–261(2018).
[6] N.I. Lebovka, L.A. Bulavin, I.A. Melnyk, K.F. Repnin, V.I. Kovalchuk, Ukrainian Journal of Physics, **60**, 910–916 (2015).

7-6.P

ELECTROKINETIC POTENTIAL AND FLOCCULATION OF KAOLIN AND BENTONITE PARTICLES BY POLYELECTROLYTES AND THEIR MIXTURES

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Polymers are widely used for regulation of the suspensions stability in many industrial applications, such as mineral processing, papermaking, water treatment. etc. In recent years there has been considerable interest in the use of multi-component flocculants, i.e. dual-polymer systems. In the latter case, due to synergetic effects, there can be significant advantages over the use of single polymers. The effect of polymers on dispersion stability is determined by the structure of adsorbed layers formed and its effect on the parameters of the electrical double layer (EDL) Measurements of the electrokinetic potential of dispersed particles in polyelectrolyte (PE) solutions provide information about changes in the EDL structure and contribution of electrostatic and non-electrostatic forces in the mechanism of flocculation of dispersions having adsorbed polyelectrolytes or their mixtures.

We have studied the effect of adsorption of anionic and cationic PEs and their binary mixtures on the electrokinetic potential, kinetics of aggregation, size and strength of flocs formed from kaolin and bentonite particles as a function of the polymer dose, charge density (CD) of the polyelectrolyte, mixture composition, sequence of the components addition and intensity of stirring the system.

It has been shown that addition of increasing amount of anionic polyelectrolytes increases the absolute value of the negative zeta-potential of particles; this increase is stronger the CD of the polyelectrolyte and pH of the system are higher. Adsorption of cationic polyelectrolytes results in a significant decrease in the negative ζ-potential and overcharging the particles surface; changes in the ζ-potential are more pronounced for samples with higher CD and at lower pH values. In mixtures of cationic and anionic PEs, in a wide range of their composition, the ζ-potential of particles is determined by the adsorbed amount of the anionic polymer independently of the CD of polyelectrolytes and the sequence of addition of the mixture components.

Maximal aggregation of suspension particles occurs at polymer content of about 0.5-1.5 mg/g that is approximately an order of magnitude less than the concentration corresponding to adsorption saturation for cationic polymers and 2-3 times less than that for anionic PEs. A synergism of flocculation capacity in mixtures of moderate and weakly charged polyelectrolytes was observed. Mixtures of medium/low charged anionic and cationic polyelectrolytes give optimum flocculation at mass ratios, corresponding to many-fold excess of negative charges over positive ones in the adsorbed layer. The laws observed were explained by features of macromolecules conformation in adsorbed mixed polyelectrolyte layers.

The research was carried out in the framework of the GINOP-2.3.2-15-2016- 00010 “Development of enhanced engineering methods with the aim at utilization of subterranean energy resources” project of the Research Institute of Applied Earth Sciences of the University of Miskolc in the framework of the Széchenyi 2020 Plan, funded by the European Union, co-financed by the European Structural and Investment Funds.

INHIBITION OF PROTEIN AMYLOID FORMATION BY CERIUM OXIDE NANOPARTICLES

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Cerium oxide nanoparticles (CeO_2-NPs) have received much attention in the biomedical field, particularly due to their antioxidant properties [1]. Oxidative stress and amyloid fibril formation are associated with the initiation and promotion of number neurodegenerative diseases [2]. The pathogenesis of these and other neurodegenerative diseases remains unclear, and effective treatments are currently lacking. The aim of this study was to examine the effect of CeO_2-NPs on amyloid fibril formation of insulin and lysozyme. CeO_2-NPs were synthesized by precipitation from reversal microemulsions based on Triton-X 100. Obtained powder had crystalline structure after synthesis. According to TEM data, CeO_2-NPs had small sizes (8 -10 nm) and were non-agglomerated. Both, insulin and lysozyme belong to the group of model proteins that may aggregate into β-sheet-rich amyloid structures. Atomic force microscopy (AFM) and Thioflavin T (ThT) fluorescence assay have been employed to investigate the amyloid aggregation of proteins in presence of CeO_2-NPs. We have demonstrated that fibrillization of insulin and lysozyme is inhibited by CeO_2-NPs in a dose-dependent manner. The apparent IC_{50} values were calculated to be ~100 μg/mL and ~ 1.53 mg/mL, for insulin and lysozyme, respectively. The disassembling effect of nanoparticles, i.e. ability to destroy pre-formed fibrils, is characterized by DC_{50} values of 213 μg/mL and 0.7 mg/mL, for insulin and lysozyme, respectively. AFM analysis fully supports ThT fluorescence study. Although the exact mechanism of protein-nanoparticles interaction is not understood, our findings may stimulate further experiments to elucidate the molecular details of the nanoparticle effect and enhance our understanding of the fibrillization process.

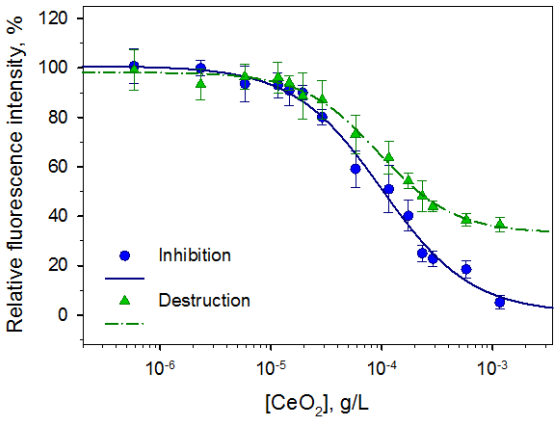

Figure 1. Monitoring of cerium oxide nanoparticles–induced inhibiting of insulin amyloid fibrillization (blue color) and disassembling of preformed insulin fibrils (green color) by ThT fluorescence assay.

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References:

[1] Estevez, A. Y. and Erlichman, J. C.Nanomedicine, 9, 1437–1440 (2014).
[2] Butterfield, D. A., Reed, T., Newman, S. F., Sultana, R. Free Radical Biol Med, 43, 658-677 (2007).

7-8.P

FREQUENCY DISPERSION OF DYNAMIC COEFFICIENTS OF VISCOSITY OF MAGNETIC LIQUIDS

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The study of viscoelastic properties of magnetic liquids (ML), allows to estimate such properties of a liquid as fluidity and compressibility, and also to describe processes of extending velocity and absorption of ultrasonic waves and others relaxation processes proceeding in the investigated liquid. Coefficients of viscosity, considering all mechanisms of an internal friction in ML are important parameters for an estimation of further use of investigated liquids in technical and industrial applications. Also, the knowledge of frequency-dependent character of change of coefficients of viscosity, allows to estimate the reaction of investigated ML on external influences.

In this connection, the purpose work is numerical research of frequency dependence of dynamic coefficients of bulk and shear viscosity ML of the given by a method of the kinetic theory. For carrying out of numerical calculations, we will use expressions for bulk $\eta_v(\omega)$ and shear $\eta_s(\omega)$ coefficients viscosity ML received in [1]. However, in [1] at numerical calculations we use of constant value of coefficient of the friction β, taken of the literary data. Actually, of friction coefficient it is closely connected with thermodynamic parameters of a condition (density, concentration and temperature). This coefficient, along with molecular parameters, in subintegral expression contains potential of intermolecular interaction and radial function of distribution. At the same time the nonequilibrium processes proceeding in a liquid are characterized by various times of a relaxation which are defined by means of friction coefficient. Therefore, we will use analytical expression of coefficient of the friction resulted in [2]. For carrying out of numerical calculations of dependence of the viskosity coefficients $\eta_v(\omega)$ and $\eta_s(\omega)$ depending on frequency, the obvious kind of potential of interaction and radial function of distribution [3] - [5], follows a choice of concrete model ML. Then expressions for dynamic coefficients $\eta_v(\omega)$ and $\eta_s(\omega)$ viscosity are assumed by the following air:

$$\eta_v(\omega)=\frac{2\pi n^2\sigma^3 kT}{9}\left[\left(\frac{1}{3}+\frac{\mu_0 M_s\tau_0\,|\vec{\nabla}H|}{\beta l}\right)\int_0^\infty drD^*(r)\int_0^r G_1(r,r_1\omega)D^*(r_1)g(r_1)dr_1-2\int_0^\infty drD^*(r)\int_0^r G_1(r,r_1\omega)g(r_1)r_1dr_1-\right.$$
$$\left.-\int_0^\infty drD^*(r)\int_0^r G_1(r,r_1\omega)g(r_1)y_2(\rho^*)r_1dr_1+\int_0^\infty drD^*(r)\int_0^r G_1(r,r_1\omega)\left[\Phi^{*L-J}(r)-\Phi^{*H}(r)\right]g(r_1)r_1dr_1\right], \quad (1)$$

$$\eta_s=\eta_{sk}(\omega)-\frac{2\pi n^2\sigma^3 kT}{45}\left(1+\frac{15\mu_0 M_s\tau_0\,|\vec{\nabla}H|}{6\beta l}\right)\int_0^\infty drD^*(r)\int_0^r G_1(r,r_1\omega)D^*(r_1)g(r_1)dr_1\,. \quad (2)$$

Results of numerical calculations for $\eta_v(\omega)$ and $\eta_s(\omega)$ depending on frequency ω, are resulted in the form of tables and drawings and also compared to experimental data. Results of the theoretical calculations spent for ML on the basis of water, will qualitatively be consistent with experimental data [6].

References

[1].Odinaev S, Komilov K, Zarifov A. // Journ. of Chem. Phys (Russ.), **82**, 6. pp. 1120-1123 (2008).
[2].Phys. of simple liquids, 1. / ed. of G.Temperli. M: "Mir", 1971, pp. 1.36-192.
[3].Ilg P., Kroger M., Hess S.//Phys. Rev., **E 71**, P. 051201 (2005).
[4].Zuowei Wang, Christian Holm, Hanns Walter Müller//Phys. Rev., **E 66**, P. 021405 (2002).
[5].Juhnovsky I.R. and Golovko M.F. The statistical theory of classical equilibrium systems. Kiev.: "Sciences dumka", 1980, 372 p.
[6].Zhiqiang Rena, Yanping Hana, Ruoyu Honga, at ell.//Particuology, **6**, P. 191-198 (2008).

7-9.P

COLORED MAGNETIC BACTERIA AND THEIR USE FOR ANIMAL FEED APPLICATION

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Currently there are no tracers that suspend stably in liquid feeds that can be easily analyzed quantitatively. In this study we developed and investigated new magnetically retrievable tracers based on magnetic bacteria *Magnetospirillum magneticum* AMB-1 colored with a food grade dye FD&C Red #3 (Erythrosin) which can be used to evaluate mixing and cross-contamination of molasses based liquid feeds, and to code critical microingredients, such as drugs and enzymes added in liquid feeds. Amount of released FD&C Red #3 in solution has been estimated using the Genesys 5 spectrophotometer at wavelength 520 nm. After performing the process of retrieving with a strong neodymium magnet, the cellular structure of colored AMB-1 was destroyed by heating with 0.5% aqueous solution of surfactant. This process released the dye from the bacteria which was then read spectrophotometrically. The homogeneity test for trial with stable suspension of Red#3-containing magnetic bacteria AMB-1 in molasses-based liquid feed was performed. The absorption values of 5 investigated solutions were obtained. It was found that a coefficient of variation (CV) for the series of sample analyses is about 10.4%. Taking into consideration the value of CV we should conclude that a mixing is complete. It is known that in order to be practically feasible ferromagnetic tracers should have the recovery at least 50%. In this respect the feasibility of proposed colored tracers based on magnetotactic AMB-1 bacteria which show a recovery of 85% of dye is obvious (the initial loading of FD&C Red #3 in molasses-based feed was as low as 5 ppm). Investigated bacteria can be used as the harmless markers (microtracers) for evaluation of mixing efficiency in liquid feeds and for qualitative and quantitative evaluation of presence of certain liquid ingredients, like enzymes, in liquid premixes and their distribution in the volume of feed.

7-10.P

DIPOLAR POLARIZATION OF PLANARLY ORIENTED 6CB LIQUID CRYSTAL WITH Cu_7PS_6 NANOPARTICLES

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The dielectric properties of planarly oriented nematic 6CB liquid crystal with Cu_7PS_6 superionic nanoparticles of the average size 117 nm has been investigated at the temperature 293 K. 6CB liquid crystals without/with Cu_7PS_6 nanoparticles were studied in a sandwich-type cell with transparent ITO electrodes. The electrodes were coated with an appropriately processed polymer layer to provide the planar orientation of the liquid crystal molecules. The cell thickness was 10 μm. The liquid crystal cell was filled using the capillary method at a temperature by 5-10 K above the nematic-to-isotropic phase transition temperature. The concentration of nanoparticles in the liquid crystal was 0.1, 0.5, 1 wt.%. The frequency dependences of the complex dielectric permittivity were measured within the frequency range 10^1-10^6 Hz using the oscilloscopic method. The influence of Cu_7PS_6 nanoparticles on the parameters of the dipolar polarization of 6CB liquid crystal molecules were studied and analysed in detail. The above mentioned polarization was revealed in the frequency range above 100 kHz. It is shown that the dipolar polarization can be described by the Debye dispersion. The time of the dipolar polarization was estimated (0.2 μs). The independence of the time of the dipolar polarization on the nanoparticles concentration was explained.

7-11.P

QUASI-MACROSCOPIC NEAR-SUBSTRATE LAYERS IN ORGANIC-LIKE LIQUIDS. THEORETICAL MODEL AND THE EXAMPLE OF NITROBENZENE

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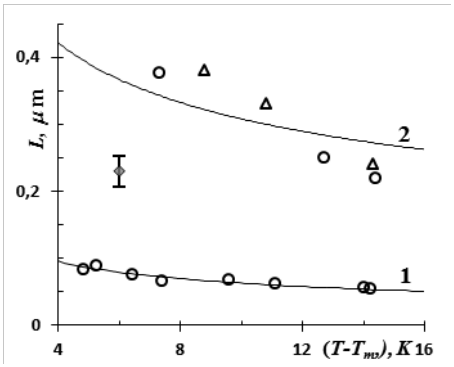
The phenomenon of molecular adsorption at the liquid/solid interface is due to the existence of a potential field extending to microscopic distances. If a liquid (as, for example, aromatic or alkane one) consists of anisometric molecules capable to association, the thickness of a boundary layer, in principle, can be many times bigger than the linear size of the molecule. Thus, the structure of the layer will resemble a uniaxial crystal (a model of the so-called epitropic phase (EP) [1]). In paper [2], a statistical model was proposed that makes it possible to express EP thickness L via temperature T and characteristic parameters of the liquid/solid interface (such as the density nad of active centers retaining the liquid molecules with the adsorption energy Wad, the association energy Wa between the liquid molecules, etc.) As the result, it turned out possible to give in [2] a satisfactory description of the experimental measurements [3] of the L(T) function for EP of nitrobenzene on quartz. In this communication we present new theoretical results concerning the statistical properties of EP allowing us to give consistent quantitative interpretation of the experimental data on the thermodynamic characteristics of sub-surface quasi-macroscopic layers in organic-like liquids. On the example of nitrobenzene, we have obtained good agreement between the theory (lines 1 and 2 in figure built with taking account of the possibility of vitrification at temperatures lower than the melting temperature Tm) and the measurements of L(T) for EP on quartz [3] (circles, the dichroism method, line 1) and on metal (circles and triangles, the optical anisotropy method, line 2) at (T–Tm) > 5 K (the experimental error is shown at the square symbol). In doing so, we used a physically reasonable idea of the form of the oligomer chain based on the structure of the molecular dimers of nitrobenzene. The difference between the theoretical predictions and the experimental data at (T–Tm) < 5 K suggests that in this region, in principle, a metastable phase of a superheated crystal could be realized. However, in order to make clear conclusions one needs more thorough experiments (they are in progress).



References

[1] B.V. Derjaguin, Yu.M. Popovskij, B.A. Altoiz. Scientific discovery of the USSR No. 388. Discoveries and inventions, No. 12, p. 1 (1991) [In Russian].
[2] B.A. Altoiz, V.N. Bondarev, E.A. Shatagina, S.V. Kiriyan, Technical Physics, 59, 1003–1006 (2014) (Zhurn. Tekhn. Fiz, 84, 58–61 (2014) [In Russian]).
[3] B.V. Derjaguin, B.A. Altoiz, I.I. Nikitenko, J. Colloid and Interface Science, 145, 441–446 (1991).

1-PENTANOL CONFORMATIONAL INFLUENCE ON VIBRATIONAL SPECTRA: FTIR INVESTIGATION IN NITROGEN MATRIX ISOLATION AND HIGH-LEVEL AB INITIO CALCULATIONS

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FTIR spectra of 1-pentanol in N2 matrix isolation were registered in wide spectral range at different temperatures. To interpret experimental results, high-level quantum chemistry calculations were performed.
41 basic 1-pentanol conformations (neglecting enantiomers) were computed using compound method ROCBS-QB3. Such approach helps authors to determine the most stable alcohol configurations. Distribution of molecular isomers in matrix isolation at different temperatures were calculated. For stable configurations (Fig. 1), dimeric cluster structures were calculated using molecular isomers in both proton donor and acceptor roles. Each next on size cluster was considered using knowledge of simpler structures stability.
Anharmonic vibrational spectra of suggested stable structures were calculated using MP2/6-311G(2d,d,p) level of theory. Further comparison of computed and experimentally measured FTIR spectra have given authors a possibility to determine cluster structure of 1-pentanol in nitrogen matrix isolation and investigate conformational influence on the clusters vibrational spectra, that results in wide spectral bands in experiment.

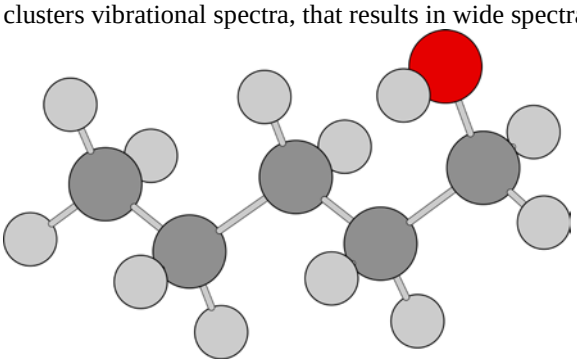

Fig. 1. The most stable configuration of 1-pentanol – TTGg conformation.

Acknowledgment
FTIR spectra of 1-pentanol in matrix isolation were registered in the Laboratory of Fourier-transform infrared absorption spectroscopy at the Vilnius University, Lithuania. The authors thank Prof. V. Balevicius and Prof. V. Sablinskas for the opportunity to perform such experiments.
Calculations of clusters (consisting of several 1-pentanol molecules) in this work were performed on the Joint ISMA/STC ISC computational cluster of SSI “Institute for Single Crystals” and Institute of Scintillation Materials NAS of Ukraine.

7-13.P

INFLUENCE OF STRUCTURAL STRESSES ON MELTING OF CRYSTALLITES OBTAINED IN POROUS MATERIALS

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The behavior feature of materials in a confined spaces is the size dependence of their physical properties. Therefore, it is possible to obtain new materials with a wide range of physical properties, changing the structure and size of nanoparticles. The nanoparticles melting point is one of the most important physical properties, because it allows to determine the damage threshold of nanostructured systems.

1-octadecene was selected, for the study of melting in crystallites, which formed in bounded space. Silica gels with different pore sizes and specific surface area were selected as a nanoporous matrix. For the study of phase transitions was used DSC apparatus Q200, TA instruments, USA.

In studying the temperature dependences of the heat flux for 1-octodecene in different porous silica gel matrices, the same phase transitions were observed as for bulk 1-octadecen. It is shown that the temperature of phase transitions decreases with decreasing pore size. The dependence of the melting point T_0 of samples on the inverse radius of pores of silica gel was constructed. (Fig. 1)

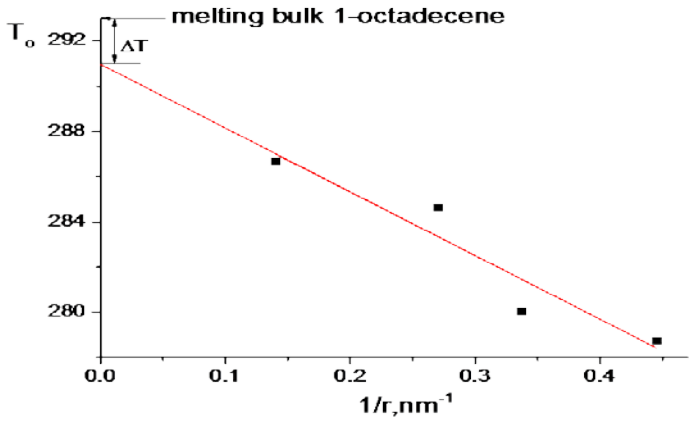

Fig. 1. The melting point dependence T_0 on the inverse radius of silica gel pores.

Structural stresses are stresses that occur during the crystallization and melting of a substance that fills the pore. These stresses have a significant effect on the melting of crystallites that form in the pores. The formula below determines the dependence of the crystallite melting temperature on the magnitude of structural stresses and the size of the crystallite.

$$T_0 = T_\infty - \frac{T_\infty}{\eta}\frac{2(\alpha_B - \alpha_A)v_A}{D} - \frac{T_\infty}{\eta}\Delta p v_A \quad (1)$$

$$\Delta T_0 = T_0 - T_\infty = \frac{T_\infty}{\lambda_f v_A}\Delta p. \quad (2)$$

The equality (2) shows that the change in the crystallite melting temperature ΔT (see Fig. 1) is due to the structural stresses Δp and does not depend on the pore size gauge. According to Figure 1, the experimental value $\Delta T = 2K$. Then we get the value of the structural stress Δp≈1 MPa.

From the studies carried out, we find that

1)structural stresses, which caused by the processes of crystallization and melting of the substance filling the pore, are about 1 MPa;

2)structural stresses change the melting point in comparison with the melting temperature of an infinite crystal. This change does not depend on the crystallite size and is about a few degrees.

SPECTRAL EVIDENCE OF THE EXISTANCE OF NANODIAMOND QUASILIQUID PHASE IN ONION-LIKE CARBON

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We carried out detailed spectral investigations of onion-like carbon (OLC) with size of ~ 20 nm, produced by powerful electric discharges (~2·104 current pulses of ~1MA magnitude) treatment of liquid and gaseous (C6H6, C6H12, C4H10, kerosene) hydrocarbons [1]. It is proved in the report, that unlike other methods of obtaining OLC (annealing of nanodiamonds, arc discharge between carbon electrodes in water, etc.), in our case a diamond-like phase with liquid-dropping core is present in a structure of the onions as a result of a high-energy input (2 MJ/l). The Raman (514.5, 325 and 257 nm) and IR absorption spectra are studied. In the Raman spectra (RS) of a large number of the samples simultaneously with the well-known fundamental G- and D ≈ G(k)- bands, additional low-frequency components D(k) and G(k') associated with vibrational states with wave vectors k at the boundary of the Brillouin zone (k'≈ k/2) are present (Fig. 1a). Detection of the bands D(k) ≈1150-1225 cm-1 proves the presence of a diamond-like phase in the produced OLC. Their existence is associated with the internal self-contraction of the onion's shells, the distance between which decreases from 0.36 nm at the periphery to 0.22 nm at the center [2]. The existence of self-contraction is proved by the displacement of D-bands to the value of ~ 1500 cm-1 in case of excitation with 257 nm, what is illustrated by the inset in Fig. 1a and enables to estimate P~ 20 GPa.

In the most studied carbon spheres, a solid diamond core is present, what is proved by the existance of a sharp D- line ~1340 cm-1 in Raman spectra. But in a number of samples, a broadened D-band ~ 297 cm-1 is observed, which can be corresponded to the liquid phase of the diamond, as it is shown in the inset in Fig. 1b. A convincing proof of the liquid-dropping shape of the diamond-like phase is the observation of overtones series of low-frequency oscillations νn=nν0 (n=2-5) of the quasi-liquid diamond shape with a solid core, which are shown in Fig. 1b. The fundamental frequency is ν0=u/cλ, where λ = 2d, d is a size of the quasi-liquid nucleus, u is the sound speed in it, and c is the speed of light. Assuming d = 2.5 nm, u = 15 km/s, we find ν0 = 100 cm-1, what agrees with the experimental value of ν0≈95cm-1. Variations of the oscillation frequencies in Fig. 1b are associated with a change of the sizes d in the samples. An important link in the developed concept is the damping of the vibration of ν0 ~ 100 cm-1, and then of the first overtone n = 2 in series 3 by a solid core.

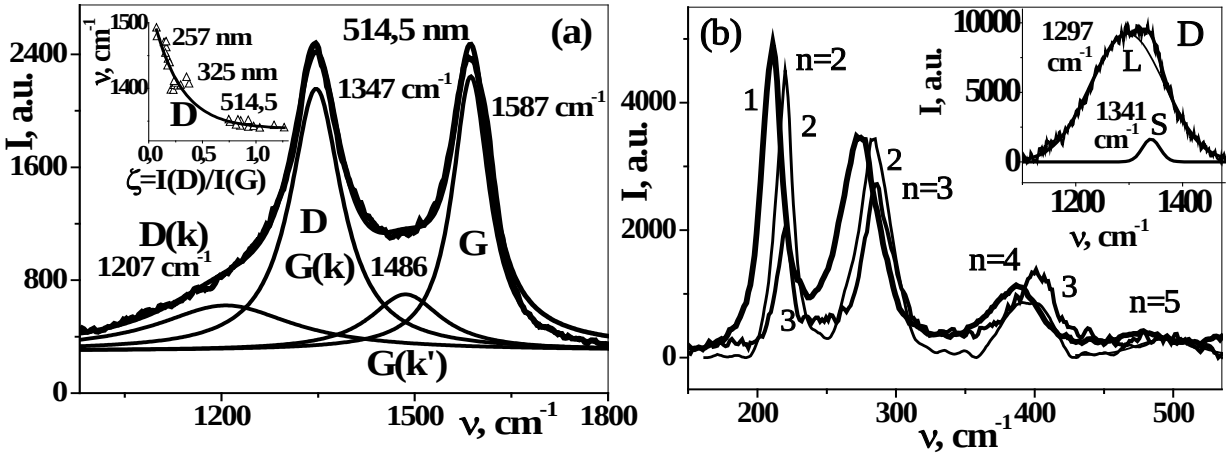

Fig. 1. Raman spectra of onion-like carbon, produced by high-voltage electrical discharge treatment of hydrocarbons

References

[1] A.D. Rud, N.I. Kuskova, V.Yu. Baklar', L.I. Ivaschuk, L.Z. Boguslavskii, I.M. Kiryan. Bulletin of the Russian Academy of Sciences. Physics, 2011, Vol. 75, No. 11, p. 1435–1441.
[2] F. Banhart, P.M. Ajayan, Nature, 1996, v.382, p.433-435.

AB INITIO MOLECULAR DYNAMICS SIMULATION OF GALLIUM CHLORIDE COMPLEXES IN FORMAMIDE SOLUTIONS

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Metal ions that selectively cleave peptide bonds under physiological conditions are promising for application in both protein bioengineering and structural studies. Recently, a number of the triple-charged metals chlorides in solutions of formamide (FA) have been investigated using standard vibrational spectroscopy techniques [1, 2]. As it follows from the presented results, stoichiometry and microscopic structure of the metal complexes in such solutions are still poorly understandable.

In the present study we perform *Ab Initio* Molecular Dynamics (MD) simulations of 1.0 molal solutions of the gallium chloride ($GaCl_3$) in FA within Born-Oppenheimer MD approach at the BLYP&TM+vdW/90 Ry level of theory using CPMD program package [3]. It was found both four- and six-coordinated $[GaCl_n(FA)_m]$ composite complexes being either positively single-charged or neutral species. Among six-coordinated complexes only *cis*- and *fac*-isomers were established as dynamically stable ones. Microscopic structure of gallium-based complexes has been analyzed in terms of radial distribution functions and corresponding running coordination numbers using MD trajectory post-processing TrAVis tool [4].

References

[1] T. B.C. Campos and W. A. Alves, *Vib. Spectrosc.*, **85**, 134-138 (2016).
[2] T. B.C. Campos, E. F. da Silva and W. A. Alves, *Vib. Spectrosc.*, **65**, 24-27 (2013).
[3] CPMD V3.13.2, Copyright IBM Corp 1990-2008, Copyright MPI für Festkörperforschung Stuttgart 1997-2001.
[4] M. Brehm and B. Kirchner, *J. Chem. Inf. Model.*, **51**, 2007-2023 (2011).

EFFECT OF ELECTROCHEMICAL CELL PARAMETERS ON THE NEUTRON REFLECTOMETRY EXPERIMENT

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Nowadays, Li-ion batteries are widely used in different electrical devices such as phones or even cars. Lithium is thought to be good material that can potentially enable the development of batteries possessing extraordinary high specific energy (e.g. lithium-metal-polymer, lithium-air or lithium-sulfur batteries). The development of high-capacity rechargeable and safe metallic lithium negative electrodes for next-generation batteries requires an in-depth understanding of reasons for nonuniform lithium plating and formation of solid electrolyte interface (SEI) during the lithium-metal battery charge. It drives the interest for the tools, enabling efficient monitoring of electrochemical interfaces, where lithium electrodeposition occurs [1,2,3].

The neutron reflectometry (NR) is one of the methods for 'in operando' study of SEI and lithium dendrites formation. The special electrochemical cell is required for such type of experiments [3]. However, there are several requirements to liquid electrolyte and solid electrodes in order to conduct a successful NR experiment.

The aim of this work is to choose optimal parameters of metal electrode and electrolyte for further NR 'in operando' research of lithium electrodeposition and study influence of roughness of SEI/dendrites layer on the NR data. For this purpose NR curves were calculated for various types and thickness of metal electrode as well as liquid electrolytes (deuterated/protonated). Thus, the obtained calculations provide a possibility to enhance the sensitivity of the NR technique to interface changes, occurring upon lithium plating. Also, models of electrochemical cell with different roughness of SEI/dendrites and cathode layer were modeled. The chi-square maps calculated to study roughness influence on data results.

References

[1] Jerliu, B., et al., (2013). Neutron reflectometry studies on the lithiation of amorphous silicon electrodes in lithium-ion batteries // Physical Chemistry Chemical Physics, 15(20), 7777-7784.
[2] Fears, T. M., et al., (2016). Evaluating the solid electrolyte interphase formed on silicon electrodes: a comparison of ex situ X-ray photoelectron spectroscopy and in situ neutron reflectometry // Physical Chemistry Chemical Physics, 18(20), 13927-13940.
[3] M.V. Avdeev, et al., Monitoring of lithium plating by neutron reflectometry, Appl. Surf. Sci. (2017).

7-17.P

DIRECTOR ORIENTATION INSTABILITY IN A PLANAR NEMATIC CELL WITH BOUNDARY CONDITION CONTROLLED BY ELECTRIC FIELD

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The planar-planar director reorientation in a nematic liquid crystal (NLC) cell in an external static electric field has been studied. The gliding of the NLC director easy axis on the polymer substrate due to the coupling between the easy axis and the electric field was taken into account.
The contribution of the coupling to the surface free energy of the system is assumed to be linear in the electric field, if the elastic fragments of substrate polymer molecules possess their own dipole moments. If the dipole moments of the elastic fragments of polymer molecules are induced by the electric field, the corresponding contribution was taken to be quadratic in the electric field. Depending on the character of the interaction between the easy axis and the electric field, the orientation instability of the director was shown to either have a threshold or not. In both cases, the dynamics of the director and the easy axis has been analyzed, by starting from the field switching-on time moment, during the transition of the system to a stationary state, and until the system returns to the initial homogeneous state after the field was switched-off.

The transmittance of the NLC cell for normally incident monochromatic linearly polarized light and its dependence of the system parameters were computed and investigated. It was shown that temporal behavior of the cell transmittance reflects the dynamics of the NLC director.

7-18.P

DIRECTOR ORIENTATION INSTABILITY OF NEMATIC LIQUID CRYSTAL IN HOMEOTROPIC CELL WITH BOUNDARY CONDITIONS CONTROLLED BY ELECTRIC FIELD

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We investigated the orientational instability of the director in a homeotropic nematic liquid crystal (NLC) cell in a dc electric field applied along or perpendicular to the cell surface depending on whether the anisotropy of the NLC static permittivity is positive or negative. The easy axis of director orientation on one of the cell surface can glide under the influence of the electric field. The contribution of a coupling between the movable easy axis and the electric field to the free energy of the system is linear or quadratic in the electric field strength depending on whether the molecules of the orientating polymer coating of the surface have permanent or induced dipole moments. In the case of NLC with positive dielectric anisotropy and the linear easy axis – electric field coupling the reorientation of the director is thresholdless. Otherwise the orientation instability of the system exhibits threshold behavior. The temporal behavior of the director field and the movable easy axis was computed for each case of NLC dielectric anisotropy and the electric field – easy axis coupling. The characteristic turn-on/off times of the system were calculated and their dependence on the cell parameters were analyzed. The values of the coefficients of the easy axis – electric field coupling and the easy axis viscosity were found from the comparison of calculated easy axis dynamics and experimental data in the case of NLC with negative dielectric anisotropy. The time dependence of the transmittance of the NLC cell for monochromatic linearly polarized light and its dependence on the parameters of the system were investigated.

SPECIAL PROPERTIES OF INTERPHASE LIQUID LAYER NEAR SOLID SUBSTRATE. ALIPHATIC HYDROCARBONS

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Special epitropic phase (EP) is formed in quasy-macroscopic liquid layers (in case of anisometric molecular shape) near solid substrate [1]. In [2] a statistical model was proposed, according to which EP is like the "pile" of molecular associates bounded by adsorption forces to the substrate. Theoretical calculation of the temperature dependence of the equilibrium EP thickness $L_S(T)$ demonstrated a good quantitative description of the experimental data in case of nitrobenzene (polar aromatic hydrocarbon). It is significant that the proposed model may be improved in order to describe the EP properties of other non-mesogenic liquids (e.g. nonpolar *n*-alkanes). The improvement is connected with the explicit introduction of the glass transition temperature T_g into the activation temperature dependence of the EP thickness (T_g has purely fluctuation nature and enters the empirical Vogel law [3]). This report presents the results of measurement of the $L_S(T)$ dependence in case of EP formed by *n*-alkane homologues and the theoretical interpretation. Fig. 1 illustrates the dependence of *n*-hexadecane layer thickness near metal substrate vs (T–T_m), where T_m is a melting temperature. The experimental data were obtained by different methods (○ - rheology [4], Δ - optical anisotropy, × - dichroism); solid line is the result of theoretical calculation, which is in good agreement with experiment in the temperature range $(T - T_m) \geq 4$ K. Fig. 2 illustrates the results of experimental measurements (**o**) and theoretical calculations (**x**) of $L_S(N)$ dependence for N=11…18 of *n*-alkanes homologues at $(T - T_m) = 9$ K. The observable increase of $L_S(N)$ correlates with the corresponding behavior in homologue molecular length and with the theoretical calculations.

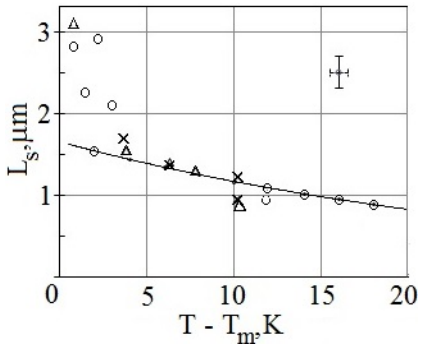

Fig. 1

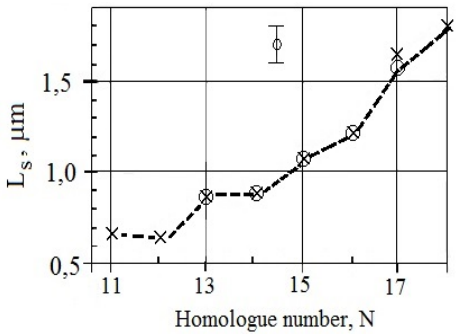

Fig. 2

References

[1] B.V. Derjaguin et al. *J. Col.&Interf. Sci.*, **148**, 56–62 (1992).
[2] B.A. Altoiz et al. *Technical Physics*, **59**, 1003–1006 (2014).
[3] L.S. Garca-Coln et al. *Phys Rev B*, **40**, 7040–7044 (1989).
[4] B.A. Altoiz et al., *Technical Physics*, **63**, 1–6 (2018).

NEW PROTON CONDUCTING MEMBRANE BASED ON BACTERIAL CELLULOSE/POLYANILINE NANOCOMPOSITE IMPREGNATED WITH PROTIC IONIC LIQUID

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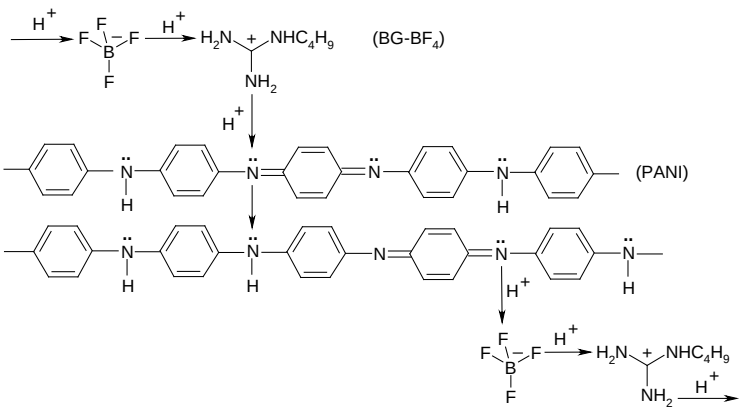
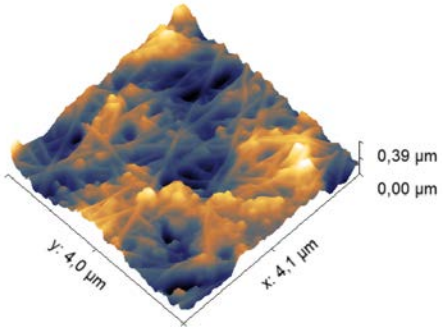
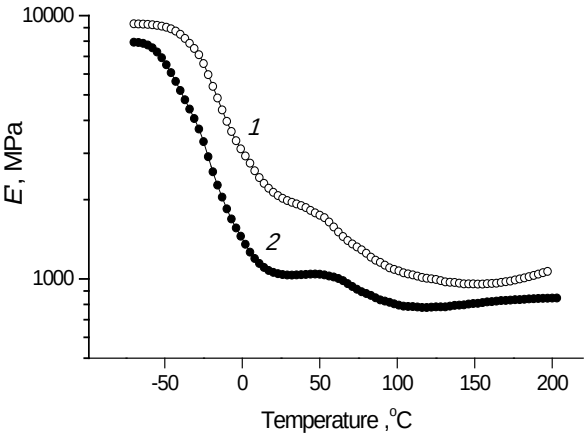
The aim of this research was to develop cheap alternative polymer-electrolyte membrane for fuel cells operating at temperatures above 100 °C. New protic ionic liquid, namely 1-butylguanidinium tetrafluoroborate (BG-BF_4) has been synthesized by simple method. The results of electrochemical impedance measurements indicate on excellent ionic conductivity of BG-BF_4 reaching the value of 0.1 S/cm at 120 °C. The natural polymer bacterial cellulose (BC) was used as a matrix for the impregnation with protic ionic liquid. Moreover, solid state proton conductor, polyaniline (emeraldine base, PANI) was deposited on the surface of BC nanofibrils by in situ polymerization of aniline. Thus, composite membrane containing 7 wt.% of PANI and 80 wt% of BG-BF_4 has been prepared. The composite membrane containing 7 wt.% of PANI and 80 wt% of BG-BF_4 reached good level of ionic conductivity above 10^{-3} S/cm in the temperature range from 100 to 180 °C. The ability of PANI to accelerate proton transfer in the ionic liquid medium has been supposed. According to dynamical mechanical analysis (DMA) data, BC/PANI/BG-BF_4 composite has high values of storage modulus from 2000 MPa at room temperature to 1000 MPa at 180 °C.



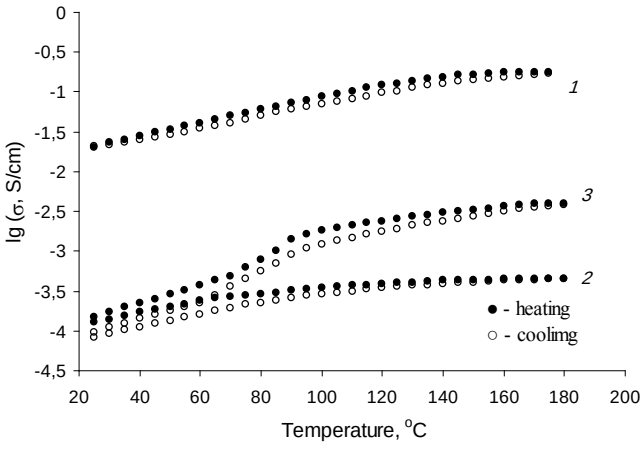
Proton conduction mechanism in BC/PANI/BG-BF_4 composite



AFM topographical image of BC/PANI/BG-BF_4 composite



DMA curves of storage modulus (E') for BC composite membranes: 1 - BC/BG-BF_4 (80%), 2 – BC/PANI/BG-BF_4 (80%)



Temperature dependences of electrical conductivity at 1 kHz: BG-BF_4 (1), BC/BG-BF_4 (80%) (2), BC/PANI/BG-BF_4 (80%) (3)

7-21.P

PLANE DIRECTOR PROFILES IN BOUNDED NEMATIC LIQUID CRYSTALS WITH STRUCTURE DEFECTS

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We use an improved conformal mapping technique to calculate analytically two-dimensional profiles of the nematic liquid crystal (NLC) director in an NLC cell. We consider the case of the strong anchoring and the piecewise constant director pretilt on the piecewise smooth curve which bounds the cross-section of the cell. An advantage of our method in comparison with the standard conformal mapping technique is that it does not require the knowledge of the inverse mapping and the calculation of the integral in the Poisson formula. Proposed technique allows to take into account structure defects in the bulk of the NLC on the symmetry axis of the region.
As an example of how the method can be used, we find an analytical expression for the director profile in a horizontal cylindrical groove partly filled with the NLC. We consider the case where a disclination line parallel to the axis of the groove occurs in the bulk of the NLC. We calculate the equilibrium distance form the disclination line to the bottom of the groove for arbitrary height up to which the groove is filled with the NLC. We show that the disclination line lies at the centre of the NLC layer, if the thickness of the layer is small in comparison with the groove radius. As the thickness grows, the equilibrium distance from the disclination line to the bottom of the groove increases approaching the value that is approximately equal to the one third of the groove radius in the case of the full groove.

7-22.P

INFLUENCE OF THE MAGNETIC FIELD AND UV IRRADIATION ON THE STRUCTURE OF GLYSEROL

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The light-scattering of glycerol between glass walls (as simplest model system for study of a properties of liquid component for liquid lenses [1]) under the influence of UV irradiation and a magnetic field was investigated. The glycerol (AZ-16-1311 Germany) with GOST technical standards 6259-75 is used. The experimental data using nephelometry method are obtained. It is experimentally detected the difference character of light scattering at preliminary processing by heating, UV-irradiation and a magnetic field. A hypothesis has been put forward on the relationship between the temperature, UV irradiation, and the magnetic field with the structure of the layer between the solid wall and glycerol.
It is shown that the presence of constant magnetic field and UV-waves stabiliz light scattering in model system. Under such external influences, presumably, the formation of a layer between glass wall and glycerol is stabilized too. The combined effect of UV irradiation and a magnetic field for the processing of a liquid agent may be a possible method to reduce the chromatic aberration of liquid lenses [2,3].

References

[1] L.Yu.Vergun, Journal of Electrical Engineering, **vol**.5, p.349-351 (2017).
[2] S.Stallinga, J.Vrehen, J.Wals, H. Stapert, and E. Verstegen, Proceedings of SPIE 48: 50-9 (2000).
[3] L.Yu.Vergun, Book of Abstracts XXII Galyna Puchkovska International School-Seminar Spectroscopy of Molecules and Crystals, p.155 (2015).

7-23.P

KINETIC PROCESSES AND DIMENSIONALITY CROSSOVER EFFECTS IN CONFINED SUPERCOOLED WATER AND NANO(MESO)SCALE LIQUIDS

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This presentation is focused at studying the following problems:

1. ***Anomalous behavior of kinetic properties (diffusion, barodiffusion, thermodiffusion coefficients, etc.) in confined supercooled water and nanoscale (mesoscale) liquids near its critical points.***

Formulae describing the dependence of diffusion, barodiffusion, and thermodiffusion coefficients on linear sizes as well as on the thermodynamic parameters (temperature, pressure, density, concentration, etc.) are analyzed in confined supercooled water (see review [1] and refs there) and nanoscale (mesoscale) liquids in three dynamic (fluctuation, crossover, and regular) regions [2-4].

2. ***Effects of dimensionality crossover on these kinetic properties of confined supercooled water and nanoscale (mesoscale) liquids.*** In particular case of $3d \leftrightarrow 2d$ dimensionality crossover [5-7,2], one has the following changes in dependence of the barodiffusivity ratio k_P on the size variable from $k_P \sim L^{1.963}$ to $k_P \sim L^{1.75}$ and on the pressure variable from $k_P \sim (p - p_c)^{-0.791}$ to $k_P \sim (p - p_c)^{-0.933}$. The same result will be valid for the temperature dependence of the thermodiffusivity ratio k_T at such a $3d \leftrightarrow 2d$ dimensional crossover.

3. ***Pecularities of the light molecular scattering spectra in nanoscale (mesoscale) liquids.*** Results, obtained above in considering a previous problem, are used for consistent studies of the dynamic light scattering in confined liquids with taking into account not only the contribution from the diffusion effect given by the Fick law but also the thermal diffusivity contribution given by the Soret effect [8-12].

References

[1] P. Gallo et al., Chem. Rev. **116**, 7463, (2016)
[2] L.A. Bulavin and A.V.Chalyi (eds.), *Modern Problems of Molecular Physics*, Springer Proceedings in Physics **197**, 253, (2018)
[3] A.V. Chalyi et al., Ukr. Fiz. J. **55**, 1113, (2010)
[4] A. Onuki, J. Chem. Phys. **85**, 1122, (1986)
[5] M.O. Kimball, K.P. Mooney, F.M.Gasparini, Phys. Rev. Lett. 92, 15301, (2004)
[6]. A.V. Chalyi, et al., Condens. Matter Phys. **16**, 23008, (2013)
[7] A.V. Chalyi, in *Physics of Liquid Matter: Modern Problems*, ed. by L. Bulavin, N. Lebovka (Springer, Switzerland, 2015)
[8] M.A. Anisimov et al., Phys. Rev. E **57**, 1946, (1998)
[9] B.W. Law, J.C. Nieuwoudt, Phys. Rev. A **40**, 3880, (1989)
[10] B.J. Askerson, H.J.M. Hanley, J. Chem. Phys. **73**, 3568, (1980)
[11] R.D. Mauntain, J.M. Deutch, J. Chem. Phys. **50**, 1103,(1969)
[12] A.V. Chalyi, V.P. Lukomskii, I.S. Gandzha, Ya.V. Tsekhmister, K.A. Chalyy, *Non-Linear Processes in Physics: Oscillations, Waves and Self-Organization* (Chetvertaya Khvylja, Kyiv, 2004).

Section 8. Nanodrops and Nanobubbles

Poster session

8-1.P

THE OBSERVATION OF LARGE SCALE NANOPARTICLES IN TRUE SOLUTIONS OF DYES *n*-DECYLFLUORESCEIN AND *n*-DECYLEOSIN

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The indicator dyes *n*-decylfluorescein and *n*-decyleosin are common molecular probes for the investigation of colloidal particles such as surfactant micelles or bilayers because of their ability to penetrate into the Stern layer due to long hydrophobic "tails". Within the course of this study, however, we examined the behavior of these dyes in surfactant-free aqueous solutions with some addition of ethanol.

In 5×10^{-6} M solution of *n*-decylfluorescein with 10% (v/v) ethanol or *n*-decyleosin with 5% (v/v) ethanol, the particles with size of about 90 – 170 nm (Z-average diameter, PdI around 0.3) were obtained at different pH values by dynamic light scattering method using Zetasizer Nano ZS Malvern Instruments apparatus. Moreover, increase in the ionic strength up to I = 0.15 M (NaCl) leads to rise of measurement quality (PdI = 0.16 ± 0.02). Relatively small polydispersity coefficients of about 0.1 – 0.2 have pointed to presence in the solution some particles, which presumably can be nanobubbles. Note, that in the absence of the dyes, the polydispersity increases strongly, and the measurement quality is much poorer. The influence of butanol-1, tetra-*n*-butylammonium iodide and NaCl as well as *n*-decylfluorescein concentration and pH on particles size and ζ-potential was investigated.

Hence, the existence of nanobubbles stabilized by both dyes and ethanol seems to be probable. At first, the distributions by intensity, by number and by volume are similar (and PdI values are low) that pointed at spherical form of particles in solution. Secondly, we observed absorption spectra which are typical for dyes in monomeric form. Consequently, the particles which observed by dynamic light scattering method using are not aggregates of dye molecules. Finally, the value of the ζ-potential of these particles is depended on the pH of buffer solutions: +15.0 ± 1.8 mV (pH = 1.97), –2.9 ± 1.0 mV (pH = 3.54), –1.1 ± 0.2 mV (pH = 4.0), –38 ± 7 mV (pH = 6.0), and –38 ± 6 mV (pH = 8.0). Moreover, the indices of the apparent ionization constants, pK_a^{app}, for the ionization of neutral form of indicator is similar to that one observed in anionic surfactant micelles, whereas the pK_a^{app} for the cationic form is similar to that in cationic micelles. Obviously, the dye molecules are situated on air – water surface of nanobubbles together with ethanol molecules and cause the charge of the bubbles.

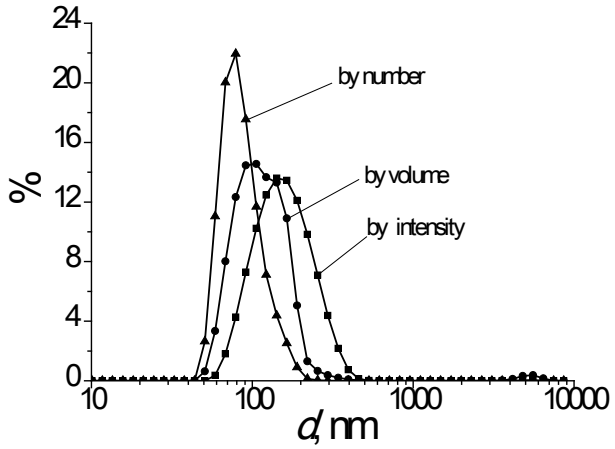

Fig. 1. The particles size distribution in 5×10^{-6} M solution of *n*-decylfluorescein with 10% (v/v) ethanol at pH of about 11.0 at I = 0.15 M (NaCl).

EVAPORATION OF BIOFUEL MULTICOMPONENT DROPLETS

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The paper presents the results of theoretical and experimental studies of evaporating individual droplets of ethanol(E), buthanol(B) and their mixtures at masspart (E) – 60%. The appearance of effective technologies for the synthesis of renewable fuels *f*rom biomass opens the new possibilities *for* the use of these alcohols as alternative fuels. In practice, alternative fuels are used as components for mixture with fossil fuels. One of the main problems lies in difference of biofuels thermophysical properties and ones for fossil fuels while attempting to increase part of biofuel additions into mixture with *transport* fuels. These features substantially influence on characteristics of drop evaporation, formation, ignition and combustion of the modified air – fuel mixture in a combustion chamber. The fuel drops evaporation as the initial stage of combustion in the engine chamber determines efficiency of all other processes. Therefore, the studies of biofuel drop evaporation and ones for their mixtures are relevant.

Theoretical studies of drops evaporation process of liquid fuels mixture in the hot air were conducted at the using discretely – component approach [1,2]. System of heat and mass exchange equations for the liquid fuel drop is including of (i+1) equations:

$$\dot{m}_i = \pi d \cdot Sh \cdot \rho_g \cdot \varepsilon_i D_i \, ln(1 + B_{M,i}); \quad (1)$$

$$\rho_l c_l \frac{dT_l}{dt} = \alpha(T_\infty - T_l)\frac{S_l}{V_l} - \frac{1}{V_l}\sum_i \dot{m}_i L_i \cdot \quad (2)$$

Here, an index i is number of mixture's components, g, l – indexes for gas and liquid phases, consequently; $\dot{m}_i$ – the vapour flow; d – the droplet's diameter; D_i – the fuel vapour diffusion coefficient; ρ_g – the air density; L_i - the specific heat of vaporization; ε_i – the component's rate into the mass flow; $B_{M,i}$ – the mass-transfer Spolding's number.

The evaporation of biofuel binary mixture droplet with mass rate of 60% (E) – *was seen as a*n example for solution of (1) and (2) equations. The dependence $d^2(t)$ was obtained for the droplet of such binary fuel's mixture (fig.1.a) and droplet's temperature behavior (fig.1.б) in the temperature interval $T_\infty = 440 - 675$ K

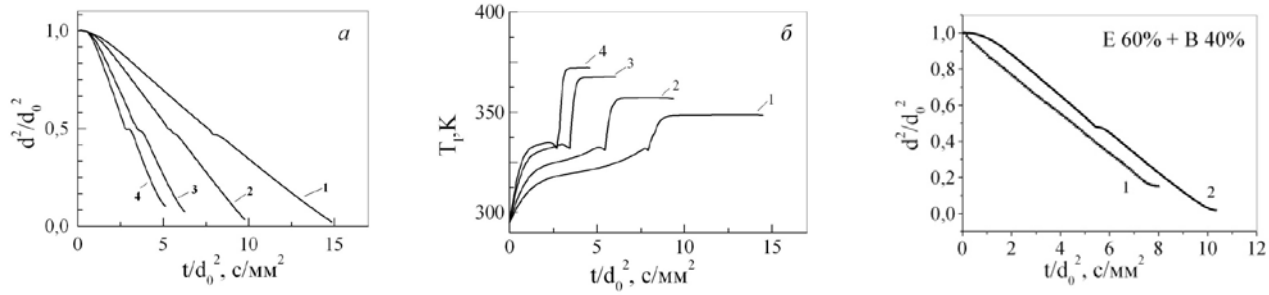

Fig.1. Evaporation kinetics of biofuel mixture droplet E 60% + B 40% and behavior of droplet's temperature. (1) – 440K, (2) – 500K, (3) – 605K, (4) – 675K.

Fig.2 Evaporation kinetics of biofuel E60%+B40% at T_∞ = 500K.. (1) – experiment, (2) – calculation.

Evaporation kinetics experimental study of single-component biofuel droplets of (E), (B) and their E60%+B40% mixtures were held in the heated air environment in the temperature range of 350÷700K and atmospheric pressure. The suspended drop's method was used.

The analysis of dependence $d^2(t)$ allowed to *obtain* the evaporation constant values of droplets both for single-component biofuels and for their mixture. The experimental values of evaporation constants correlates with calculations data (fig.2). The absence *of special areas* (nonlinear areas) in experimental data, which are present in calculation results (fig.2), may be explained by the thermal influence of suspension - the fact that was not taken into account while modelling.

References

[1] Sazhin S.S. Advanced models of fuel droplet heating and evaporation // Progress Energy and Combustion Science. – 2006. – Vol. 32. – P. 162 - 214.

[2] Zhang L. Vaporization modeling of petrolium-biofuel drops using a hybrid multi-component approach // Combustion and Flame. – 2010. – Vol. l57. – P. 2165-2174.

Section 9. Phase transitions and critical phenomena in liquids and liquid systems

Oral session

9-1.O

A MESOSCOPIC THEORY OF HETEROPHASE FLUID IN APPLICATION TO THE GAS-LIQUID AND METAL-NONMETAL TRANSITIONS IN EXPANDED MERCURY

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The fluid states of mercury are described in the framework of a mesoscopic theory of a 3-phase random mixture of mutually transforming fluctuons. Fluctuons represent the liquid-like-metallic, liquid-like-nonmetallic, and gas-like elementary species of the fluid. Formulated free energy of the system of interacting fluctuons produces a thermodynamic equation of state. It is found that for an appropriate set of parameters both the vapor-liquid transformation and the metal-nonmetal transformation in the liquid phase of mercury are accurately described. The solutions of the equation of state explain the nonlinearity and asymmetry of the diameter of the liquid-vapor coexistence curve and reveal the physics of metal-nonmetal transition. It is shown shown that the observed dielectric anomaly in mercury is induced by an excitonic transition at the percolation threshold of the nonmetallic liquid fraction. The partial conductivities and dielectric permittivities of gas phase, as well as metallic and nonmetallic liquid phases are determined. The phase diagram of mercury with its continuous and discontinuous transformation lines is reproduced.

9-2.O

ANOMALOUS DYNAMIC PROPERTIES OF BINARY SOLUTIONS NEAR THEIR SINGULAR POINTS

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The thesis studies anomalous dependence of dynamic viscosity, effective absorption coefficient and sound propagation in different thermodynamics areas: phase transition, critical isotherm and isoconcentration. Here with binary solutions were studied near different singular points: phase separation of molecular, ion-molecular, ion-electronic binary solutions; and 1,2-propanol-water alcohols solutions near structural phase transition. Contrary to the existing assumptions of dynamic scaling theory, available to monitor experimental conditions showed that fluctuation part is less than the regular one for the value of dynamic viscosity and sound absorption coefficient.

The conclusion of scaling transformations finite-size theory on finite viscosity value and sound absorption coefficient at critical values of $x=x_c$ concentration and $T=T_c$ temperature is confirmed. The conducted acoustic research in a wide range of frequencies, (5-2500) MHz, for the first time allowed to propose the method of evaluation the contribution to effective sound absorption coefficient, which is connected with anomalous scattering of sound at concentrations fluctuations both near the critical point of phase separation and singular point of water-alcohol solutions. It is shown that H-bonds are responsible for the observed water and aqua structural phase transition. In the studied 1,2-propanol–water the transition occurs in the vicinity of 42^0C when water changes its structure. Temperature and concentration of water solutions singular point is defined as the intersection point of corresponding curves of temperature or concentration dependence of sound velocity and absorption coefficient. Based on the analysis of temperature dependences of sound propagation velocity and absorption coefficient, the method allowing to estimate lifetime of concentrations fluctuations in the studied binary solutions with critical concentration when approaching the critical point of homogeneity is proposed.

It is determined that the time of equilibrium establishing in water-alcohol solutions in the vicinity of liquid-liquid structural phase transition is much more then the time of equilibrium establishing in binary solutions with the phase separation critical temperature. This is the key difference of mesoscale liquid-liquid structural phase transition from the critical phase separation in binary solutions. It is found that theory of dynamic critical phenomena describes sound coefficient and propagation velocity anomalies connected with concentrations fluctuations or structural changes only in fluctuation area of $\omega\tau_{fl}>>1$ frequencies. Increase of frequency as well as deviation from critical temperature or concentration brings the system to crossover or even hydrodynamic area.

9-3.O

THE EQUATION OF STATE IN THE SUPERCRITICAL REGION AND THE WIDOM LINE OF A FLUID MODEL

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We propose the analytic method for the derivation of the state equation of a fluid model [1] in the region above the critical temperature ($T>T_c$), which is elaborated using the renormalization group transformation in the collective variables set in the framework of the grand canonical ensemble. The constituents of the system interact via the Morse potential. Mathematical description with allowance for non-Gaussian fluctuations of the order parameter is performed in the vicinity of the critical point on the basis of the quartic measure density (the ρ^4-model). The recurrence relations between the coefficients of effective non-Gaussian measures of density, the solutions of these relations and the equation for a phase transition temperature are derived. The total expression of the thermodynamic potential in case of temperatures $T>T_c$ is obtained as a compilation of terms derived for each fluctuation regime. The equation of state with fluctuational effects taken into account is derived for the cases of $T>T_c$ and $T=T_c$. The proposed method of calculation of the grand partition function allows deriving the critical temperature, the critical indexes of the correlation length, the isothermal compressibility. This method also enables deducing the expression for plotting the Widom line [2] directly from the equation of state.

References

[1] Kozlovskii, M. P. and O. A. Dobush, Condens. Matter Phys., **20**.2 (2017): 23501-23519
[2] Artemenko, S., P. Krijgsman and V. Mazur, J. Mol. Liq., **238** (2017): 122-128

9-4.O

LANDAU-GINSBURG KINETICS OF GRANULAR FLUID COMPACTION

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Granular fluid is a subject of intensive studies in the soft matter physics [1]. Structurization in form of formation of specific domains which has an individual symmetries are known either from experiments [2] or from theoretical modeling [3-7]. It has been shown that granular fluids can be characterized by non-trivial differential equation of state which in general takes a form of Abelian equation [3].

In the present paper Landau-Ginsburg formalism has been applied to study the kinetics of structural transformation in externally perturbed granular fluids. The relevant relaxation law for selected order parameter was investigated in the close vicinity of crystallic ordered phase (which is observed experimentally [2]). It is shown that of these mechanical process has a characters of first-order phase transitions.

Landau-Ginsburg kinetic equation describing the relaxation of compaction to the asymptotic quasistationary state has been formulated. We obtain analytical solutions, which describe relaxation of the relevant order parameter field in a sequential piecewise set of intervals of the values of packing parameter. The obtained results agreed with the data of measurements concerned the compaction in granular materials subjected to external perturbation field.

References

[1] O.I. Gerasymov, *Physics of granular materials* (TES, Odesa, 2015).
[2] N. Vandewalle, G. Lumay, O. Gerasimov and F. Ludewig, *Eur. Phys. J. E*, **22**, 241-248 (2007).
[3] O.I. Gerasimov and P. Schram, *Physica A*, **312**, 172-180 (2002).
[4] O.I. Gerasimov, P.P.-J.M. Schram and K. Kitahara, *Ukr. J. Phys.*, **48**, 885-896 (2003).
[5] O.I. Gerasymov, *Ukr. J. Phys*., **55**, 560-567 (2010).
[6] O.I. Gerasymov, N.Vandewalle, A.Ya. Spivak, N.N. Khudyntsev, G. Lumay, S. Dorbolo and O.A. Klymenkov, *Ukr. J. Phys*., **53**, 1128-1135 (2008).
[7] O.I. Gerasymov and A.Ya. Spivak, *Ukr. J. Phys*., **60**, 253-257 (2015).

9-5.O

NONLINEAR DYNAMICS OF ICE SURFACE SOFTENING AT FRICTION WITH A GLANCE OF NOISE

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For the description of ice surface softening by friction the viscoelastic model of medium with heat conductivity is elaborated. The premelting is construed by the Kelvin-Voigt equation for shear strain and by the relaxation equations of Landau-Khalatnikov-type for shear stress and temperature. Considering the additive non-correlated fluctuations of the shear strain and stress, and the temperature in these equations the Langevin and Fokker-Planck equations are derived. Their analysis is based on the investigation of extrema of the distribution function, i.e., steady state values of the shear strain, using the Stratonovich interpretation. The phase diagrams are constructed, where the noises intensities and thermostat temperature determine the regions of crystalline and softened ice, as well as their mixture (*stick-slip* rubbing). We present that domain of crystalline ice friction is bounded by relatively small background sliding block temperatures and fluctuations intensities of the stress and temperature.
The Euler method is used for numerical solution of Langevin equation. The calculated friction force time series are compared with experimentally observed ones for rubbing of a polymer (poly(methyl methacrylate) PMMA), rubber and steel on ice as well as polycrystalline freshwater and saline ice over itself. The time series of different modes specify the different friction regimes in accordance with rubbing force probability distributions. The friction force value, which is close to zero, is realized at ice friction regime. The casual transitions between zero and non-zero rubbing force values occur at *stick-slip* regime. The softened ice regime is characterized by positive friction force always. The fast Fourier transform analysis of the time series gives a spectrum of the friction force oscillations. The typical spectrum approximation line $S_p(\nu) \propto 1/\nu^{0.85}$ has falling form with the frequency ascent that contradicts to the white noise property $S_p(\nu)$ = const. Consequently, the different time correlations are present in the model.

9-6.O

LOW-TEMPERATURE GLASSY ANOMALIES IN THERMAL PROPERTIES OF MOLECULAR SOLIDS

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It is of the uttermost interest to understand the nature of glassy thermal anomalies in disordered molecular crystals and solids, which are usually at low temperatures. In recent years, new experimental data were obtained on the dominant role of rotational degrees of freedom in the low-frequency dynamics of disordered crystals [1.2]. In this review, we highlight the role of different molecular disorder types of materials consist of globular or cyclic molecules. We also discuss new correlations between position of Boson peak and non-acoustic excitations contribution to heat capacity and thermal conductivity. Our findings help for understanding the origin of the controversial topic of low-temperature glassy properties.

References

[1] T Romanova, P Stachowiak, A Jeżowski, AI Krivchikov, GA Vdovychenko *Physica B:* **459**, 93-96 (2015).
[2] J. F. Gebbia, M. A. Ramos, D. Szewczyk, A. Jezowski, A. I. Krivchikov, Y. V. Horbatenko, T. Guidi, F.J. Bermejo, and J. L. Tamarit, *PRL*, **119(21)**, 215506. (2017).

NON-PHOTOCHEMICAL LASER-INDUCED NUCLEATION

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Non-photochemical laser-induced nucleation (NPLIN) was discovered in 1996 [1]. Nanosecond pulses of near-infrared or visible laser light cause rapid crystallization in supersaturated solutions, despite the solutions being transparent at the laser wavelengths [1-4]. NPLIN can be understood with classical nucleation theory by including a decrease in bulk free energy arising from electronic polarization of solute clusters by the laser electric field [2-4]. At least three observations remain unexplained: there is a threshold laser intensity for NPLIN; the laser pulse duration must be at least 100 ps to cause NPLIN; and the NPLIN rate is increased by adding impurity nanoparticles [5]. Molecular dynamics (MD) simulations of supersaturated KCl(aq) show that the residence time of ions in amorphous clusters is 10-100 ps, and that the collective ion dynamics are 'glassy' [6]. If the cluster reorganization time is 10-100 ps, then the laser pulse should be of at least that duration for NPLIN to occur, which agrees with the experimental observations. Impurity nanoparticles could absorb the laser light, leading to localized heating of the solution. MD simulations of a carbon-like nanoparticle in supersaturated NaCl(aq) show that, 2-3 ns after heating, ions are concentrated and strongly clustered 15-20 Å from the nanoparticle surface [7]. Nanoparticle heating might therefore dictate the observed threshold laser intensity.

References

[1] B. A. Garetz *et al.*, *Phys. Rev. Lett.* **77**, 3475-3476 (1996).
[2] A. J. Alexander and P. J. Camp, *Cryst. Growth. Des.* **9**, 958-963 (2009).
[3] C. Duffus *et al.*, *J. Am. Chem. Soc.* **131**, 11676-11677 (2009).
[4] M. R. Ward and A. J. Alexander, *Cryst. Growth Des.* **12**, 4554-4561 (2012).
[5] M. R. Ward *et al.*, *Cryst. Growth Des.* **16**, 6790-6796 (2016).
[6] J. O. Sindt *et al.*, *J. Phys. Chem. B* **118**, 9404-9413 (2014).
[7] J. O. Sindt *et al.*, *J. Chem. Phys.* **147**, 214506 (2017).

TO LANDAU DEFINITION OF EFFECTIVE HAMILTONIAN IN HIS THEORY OF PHASE TRANSITION

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Landau theory of phase transitions of the second kind is completely phenomenological one and is based on his expression for non-equilibrium thermodynamic potential that is a function of order parameters η_a. This potential is given by an expansion in a series in powers of the parameters η_a because at the transition point these parameters are small. In the Landau expression terms up to the forth powers of η_a are kept and coefficients of the expansion are considered as phenomenological functions of temperature T with some necessary properties.
In non-published definition given by Pitaevsky in book [1] Landau proposed to start from equilibrium distribution for the order parameter

$$w(\eta) = \mathrm{Sp}\, w\delta(\eta - \hat{\eta}); \qquad w = e^{\frac{F-\hat{H}}{T}}, \qquad \mathrm{Sp}\, w = 1; \qquad \delta(\eta - \hat{\eta}) \equiv \prod_a \delta(\eta_a - \hat{\eta}_a); \tag{1}$$

were w is the Gibbs distribution, F is equilibrium free energy, $\hat{H}$ is Hamiltonian of the considered system. Then non-equilibrium free energy $F(\eta)$ is defined by the Boltzmann formula

$$w(\eta) = e^{\frac{F-F(\eta)}{T}}. \tag{2}$$

with the full equilibrium free energy F. So, Landau proposed to restrict ourselves by non-equilibrium states which coincide with states observed in equilibrium fluctuations. Distribution (2) is a complete analog of the Gibbs distribution. Therefore, Landau proposed to call function $F(\eta)$ the effective Hamiltonian of the system in space of variables η_a. However, Landau did not realize his definition in a microscopic theory.
In the present paper the Landau effective Hamiltonian $F(\eta)$ is calculated for an isotropic system close to the equilibrium, when deviations $\delta\eta_a = \eta_a - \eta_a^0$ of the order parameters η_a from their equilibrium values $\eta_a^0 = \mathrm{Sp}\, w\hat{\eta}_a$ are small, that gives

$$F(\eta) = F + \frac{3T}{2}\left(\ln\frac{2\pi\langle\hat{\eta}^2\rangle}{3} - \frac{3}{4}\frac{\langle\hat{\eta}^4\rangle}{\langle\hat{\eta}^2\rangle^2}\right) + \frac{3T}{2\langle\hat{\eta}^2\rangle}\left(1 + \frac{3}{2}\frac{\langle\hat{\eta}^4\rangle}{\langle\hat{\eta}^2\rangle^2}\right)\delta\eta^2 - \frac{27T}{40}\frac{\langle\hat{\eta}^4\rangle}{\langle\hat{\eta}^2\rangle^4}\delta\eta^4 + O(\delta\eta^6). \tag{3}$$

Here $\langle\eta^2\rangle$, $\langle\eta^4\rangle$ are equilibrium correlation functions ($\eta^2 \equiv \eta_n\eta_n$, $\eta^4 \equiv (\eta^2)^2$) and additionally it is assumed that higher correlation functions $\langle\eta^{2s}\rangle$ ($s \geq 2$) are small and the function $\langle\eta^4\rangle$ is taken into account in the linear approximation (so, parameter $\langle\hat{\eta}^4\rangle / \langle\hat{\eta}^2\rangle^2$ is considered as a small one).

References

[1] L.D. Landau and E.M. Lifshits, Statistical Physics. Part 1, Oxford, Pergamon Press, 1980, 544 p.

SELF-CONSISTENT STATISTICAL THEORY OF CRITICAL PHENOMENA IN LENNARD-JONES FLUID

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Creation of a consistent theory of critical phenomena, free of far-reaching hypotheses, is still an actual problem of fundamental physics. The derivation of a correct equation of state for fluid requires the knowledge of its pair correlation functions (PCF) near the critical point. However, with the today possibilities of the computer simulations, the numerical calculations of PCF in sufficient proximity to the critical point can hardly be realized [1]. Therefore, the reliable information about the PCF of a "critical" fluid can, in fact, be obtained only with the help of the accurate equations of the theory of fluids. In a similar way, the critical exponents for 3D fluid were calculated in [2, 3], including the exponent $n = 6/5$, which describes the asymptotic behavior of the total PCF $h_c(r)$ directly at the critical point. In [4] it was reported about the calculation of the next to the leading asymptotic terms (with exponents $n' \approx 1.735$ and $n'' \approx 2.27$) in $h_c(r)$. In the present communication, based on the results of [2–5] for the Lennard-Jones fluid, it is proposed an explicit form of $h_c(r)$ whose asymptotic behavior is described by power-type terms with the exponents n [2] and n' [4]. The proposed theory is free of any fitting parameters, since only exact relationships (including the "sum rules" [3, 5]) are used to find the shape of $h_c(r)$. As a result, *for the first time*, using the fundamental equations of the theory of fluids, a self-consistent procedure is developed to construct $h_c(r)$ and "related" PCFs, such as the direct PCF, the bridge function $B_c(r)$, and the cavity correlation function for the fluid at criticality. The calculations of $B_c(r)$ by our theory are located, as expected, "between" the data of newest simulations [1] of the bridge function on the critical isotherm for densities below and above the critical density. The obtained results demonstrate the possibility of constructing a comprehensive self-consistent statistical theory of the critical properties of real fluids.

References

[1] A. R. Saeger, J. K. Johnson, W. G. Chapman, and D. Henderson, *Mol. Phys.*, **114**, 2516–2522 (2016).
[2] V. N. Bondarev, *Phys. Rev. E*, **77**, 050103(R) (2008).
[3] V. N. Bondarev, *Eur. Phys. J. B*, **77,** 153–165 (2010).
[4] V. N. Bondarev, 7th Intern. Conf. PLMMP. May 27-30, 2016, Kyiv, Ukraine. Book of abstracts, 9-4.O, p. 176.
[5] V. N. Bondarev, *Eur. Phys. J. B*, **84**, 121–129 (2011).

COMPUTATIONAL MOLECULAR ENGINEERING BY MULTICRITERIA FORCE-FIELD OPTIMIZATION

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Reaching quantitative agreement with the available data, and predicting properties where experimental data are absent, computational molecular engineering transforms engineering data science. However, to reach the precision required by engineering applications, molecular models need to be adjusted to a variety of thermodynamic properties. This implies the presence of multiple conflicting objectives. Addressing the field of molecular model development for the quantitatively accurate reproduction and prediction of fluid properties, results are reviewed from work using the massively parallel molecular dynamics code ls1 mardyn [1, 2], facilitating simulations of systems with up to 21 000 000 000 000 molecules (world record as of 2018). For molecular dynamics simulation of vapor-liquid interfaces, a long-range correction scheme is applied to compute long-range interactions for multi-site molecular force-field models in systems with planar symmetry, combining the Janecek method with angle-averaging following Lustig [3]. In this way, the vapor-liquid surface tension of the molecular models can be computed efficiently with a high precision.

On this basis, the progress and the remaining limitations of the application of molecular modeling and simulation to vapor-liquid coexistence are discussed, in particular, concerning the accuracy of model predictions for the vapor-liquid surface tension and the potential for a further improvement by multicriteria optimization of the force-field parameters [4]. In the present work, the two-center Lennard-Jones plus point quadrupole (2CLJQ), two-center Lennard-Jones plus point dipole (2CLJD), and Mie-6 model classes are considered [5, 6], and the multicriteria optimization problem is addressed by constructing the Pareto front, i.e., the set of rational compromises, from which models tailored to special needs can subsequently be chosen consciously by individual users or automatically [7, 8], e.g., by thermodynamic property databases and simulation software. Three optimization criteria are defined by the normalized root mean square deviation for the saturated liquid density, the saturated vapor pressure, and the vapor-liquid surface tension. An approach based on self-organizing patch plots is used to visualizing the Pareto front [4]. The Pareto knee region is investigated, and model parameterizations are identified which constitute an overall compromise between interfacial and bulk properties [5].

References

[1] http://www.ls1-mardyn.de/
[2] C. Niethammer, S. Becker, M. Bernreuther, M. Buchholz, W. Eckhardt, A. Heinecke, S. Werth, H.-J. Bungartz, C. W. Glass, H. Hasse, J. Vrabec, M. Horsch, *Journal of Chemical Theory and Computation* **10(10)**, 4455 – 4464, 2014
[3] S. Werth, M. Horsch, H. Hasse, *Molecular Physics* **113(23)**, 3750 – 3756, 2015
[4] K. Stöbener, P. Klein, S. Reiser, M. Horsch, K.-H. Küfer, H. Hasse, *Fluid Phase Equilibria* **373**, 100 – 108, 2014
[5] S. Werth, K. Stöbener, P. Klein, K.-H. Küfer, M. Horsch, H. Hasse, *Chemical Engineering Science* **121**, 110 – 117, 2015
[6] S. Werth, K. Stöbener, M. Horsch, H. Hasse, *Molecular Physics* **115(9 – 12)**, 1017 – 1030, 2017
[7] S. Vafaeyan, J. Thibault, M. Titica, IFAC Proceedings Volumes 40(4), 139 – 144, 2007
[8] S. Vafaeyan, J. Thibault, *Computers and Chemical Engineering* **33(11)**, 1814 – 1825, 2009

9-11.O

SELF-ORGANIZED CRITICAL SUPERFERROMAGNETIC DYNAMICS

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Superferromagnetism (SFM) was invoked to specify the structures involving quantum confined objects, e.g., atomic clusters, quantum dots, nanocrystals referred for hereafter as, simply, NC, see [1] and refs. therein. Such system are of fundamental interest for a study of interactions, transport processes and phase features at fairly wide range of various parameters, e.g., coupling constants, densities, Coulomb blockade gaps etc. Such super-crystals allow for considerable benefits in *'figures of merits'* for technological, biological and therapeutic applications.
We consider magnetodynamics of NC arrays by employing the randomly jumping interacting moments (RJIM) model [1] including quantum fluctuations due to the dot discrete level structure, inter-dot coupling and disorder. Magnetic state equation of such a system is demonstrated to exhibit spinodal regions in *{disorder, magnetic field}*-plane and the critical points. In vicinity of such points of self-organized (SO) criticality the magnetization evolves as erratic jumps similar to the well-known Barkhausen effect. Exploring correlations of noise amplitudes represents then convenient analytical tool for quantitative definition, description and study of SO criticality in magneticNC assemblies. We find strong correlations in jump amplitude distributions characterizing, thereby, a system with respect to NCs and a disorder.

References

1. V.N. Kondratyev, *Phys.Lett.* A **354**, 217 (2006); *J. Phys. CS* **129**, 012013 (2008)

9-12.O

THE ROLE OF THERMAL TREATMENTS IN MEMORY BEHAVIOUR OF SHAPE MEMORY ALLOYS

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Heat treatment, homogenization and phase transformations have great importance in the processing of materials as a tool in industry and other field. Shape memory effect is a temperature dependent phenomenon exhibited by certain alloy systems called shape memory alloys which take place in the class of smart and functional materials, due to the response to the variation of temperature and external conditions. These alloys have dual characteristics called thermoelasticity and superelasticity, governed by thermal and stress induced martensitic transformations performed thermally and mechanically, respectively. Shape memory alloys can be plastically deformed with external stress in the low temperature product phase condition and recover the original shape on heating, and cycle between original and deformed shapes on cooling and heating, respectively. The origin of this phenomenon lies in the fact that the material changes its internal crystalline structure with changing temperature. Shape memory effect involves a crystallographic phase transformation, martensitic transformation, on cooling and reverse austenitic transformation on heating. Martensitic transformation is performed by internal stresses in the material.
Thermal induced martensite occurs as twinned martensites by means of lattice invariant shears in two opposite directions, <110 > -type directions on the {110}-type plane of austenite matrix in self-accommodating manner and consists of lattice twins. By applying external stress, the twinned martensites turn into detwinned martensites by means of strain induced martensitic transformation. The twinning occurs with internal stresses, while detwinning occurs with the external stresses. Twinning and detwinning processes can be considered as elementary processes activated during the transformation. Temperature has great importance in the thermomechanical behavior of shape memory alloys. Shape memory effect is performed in a temperature interval, whereas superelasticity is performed mechanically in a constant temperature in parent phase region, just over the austenite finish temperature. Deformation at different temperature exhibits different behavior beyond shape memory effect and superelasticity.
Copper based alloys exhibit this property in metastable beta-phase region, which has bcc based structures at high temperature parent phase field. Lattice invariant shear is not uniform in copper based alloys and cause the formation of complex layered structures, depending on the stacking sequences on the close-packed planes of the ordered lattice.
In the present contribution; x-ray and electron diffraction were carried out on two solution treated copper based CuZnAl and CuAlMn alloys. Homogenization is important for the quality of shape memory and obtained by annealing these alloys in high temperature beta-phase region. X-Ray diffraction profiles taken from the aged specimens in martensitic conditions reveal that crystal structures of alloys chance in diffusive manner. This result refers to the stabilization.
Key words: Shape memory effect, martensitic transformation, superelasticity, lattice invariant shear, twinning and detwinning

9-13.O

GLOBAL ISOMORHISM: FROM BULK TO SURFACE

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We shortly review previous [1,2] and discuss recent [3] results on the global isomorphism between fluids states of molecular fluids and lattice models. The explanation of empirical facts on the low-temperature asymptotic properties of thermodynamic quantities for the liquid branch of the bimodal is given on the basis of information on low-temperature behavior of the Ising model. The critical value of the compressibility factor Z_c is related to that of the isomorphic lattice model. The approach is applied to the study of surface tension in a whole region of liquid-gas coexistence. The relation between critical amplitudes of the surface tension of the fluid and the Ising model is derived and compared with known results. The methodology is demonstrated for the 2D LJ fluid on the basis of the exact solution of the 2D Ising model and is tested for the 3D LJ fluid. As a result, an expression for the surface tension without any fitting parameter is derived.

References

[1] Kulinskii, V. L., *J. Chem. Phys*, **141**, 054503 (2014)
[2] Kulinskii, V. L. & Maslechko, *J. Phys. Chem. C*, **120**, 8790-8803 (2016)
[3] Maslechko, A.; Glavatskiy, K. & Kulinskii, V., *Journal of Molecular Liquids* , **235,** 119 - 125 (2017).

9-14.O

THE MODEL OF LIQUIDS AS SOLIDS WITH THE SHEAR INSTABILITY

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The properties of liquid are described by the short-range order commonly. Such consideration is adequate far from the critical points.
In the present report we propose a model that can be valid near the phase transition (for example, liquid-crystalline solid). The model is based on the assumption that in the liquid state, certain characteristics inherent in the solid are preserved. In a solid (crystal), the shear elastic modulus exists, it is absent in the liquid. However, for some types of structural phase transition (PT), softening of the transverse modulus of elasticity occurs, i.e. this module decreases by orders of magnitude (shear instability). In this case 2D defects appear in the solid, breaking the long-range order. Consequently, near such a PT, the properties of a solid are close to those of a liquid. The microscopic structure of these defects (phase boundaries and stacking faults) is described in [1, 2], where it is shown that when the shear modulus decreases, the width of the defect increases, and its energy decreases. The transition to the liquid state increases the number of flat defects, and their volume reaches the volume of the ordered phase or even exceeds it. This is structurally manifested as a breaking of the long-range order. The macroscopic manifestation of this transition is the the zeroing of the shear modulus. Presence of multidirectional 2D movable defects creates the possibility of easy deformation and long-range order breaking in different directions inside the liquid.

References

[1] V. A. Lykah and E. S. Syrkin, *J. Low Temp. Phys.*, **160**, 179-194 (2010).
[2] V. A. Lykah and E. S. Syrkin, *J. Low Temp. Phys.*, **181**, 10–29 (2015).

9-15.O

CFD MODELLING OF PSEUDOCRITICAL TRANSITIONS OF SUPERCRITICAL WATER FLOWING IN CHANNELS

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This study deals with Computational Fluid Dynamics (CFD) FLUENT software investigation of pseudocritical transition in supercritical water flowing upward in bare vertical heated tube. The solution of equations system of Navier-Stokes, continuity and energy is presented. The k – ω SST turbulence model was used to solve the problem. The physical properties of supercritical water were determined according software NIST REFPROP integrated into FLUENT code. The dates comparing of CFD predictions with experimental results are given. It was shown that there was a good agreement between the compared dates along the entire length of the tube.

The motion pattern of pseudophase transition front defined by the pseudocritical temperature is discussed. TheCFD simulation was carried out at different values of heat flow on the wall (from 189 kW/m^2 to 826 kW/m^2). The data about the regularities of the beginning and the ending fronts of pseudophase transition motion corresponding to a zone ± 25 around the pseudocritical point are presented.

The features of the change in thermophysical properties of supercritical waterand their effective values along different coordinates are considered.

SYMMETRIC ALGEBRA OF FLUCTUATION VARIABLES FOR QUANTITATIVE DESCRIPTION OF EXPERIMENTAL DATA NEARBY TO THE CRITICAL POINT

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Integrated investigations of the gravity effect phenomenon by the method of molecular light scattering [1] have shown the importance of studying the equation of state for the critical fluid (CF) in the fluctuation region, not only for temperature but also for altitude-field dependences of thermodynamic quantities [2]. Until now, the feasibility of the algebra of fluctuating variables (AFV) has not been quantitatively tested in the entire close environment of critical point (CP). Its coefficients were not determined from the experimental data and their physical meaning was not connected with the properties of long-scale fluctuations of the order parameter. Therefore, the form of the AFV for the entire close vicinity of the CP remained undefined.

To solve this problem, we first proved the complete symmetry of the exact equations of thermodynamics with respect to field and density variables. It follows that in AFV there must be an equal number of field and density variables. We proposed to call such algebra as symmetric algebra of fluctuating variables (SAFV). However, this condition is not satisfied for complete scaling approach [3] which involves three field and two density variables.

Related to this task is a number of discussion issues, for example:

1. What are the forms of symmetric and asymmetric corrections to the master equation of state nearby to the CP?
2. Are the coefficients of the crossed terms of the SAFV small, as for the AFV of Pokrovskii [4]?
3. Does the rectilinear diameter have a physical meaning close to the CP?
4. Is the conformal invariance condition violated on the critical isochore [5]?
5. What is the physical meaning of the renormalization operation near the CP?

In this study were used: 1. thermodynamic data in the vicinity of CP using the example of water [6]; 2. proposed comprehensive thermodynamic formalism [7]; 3. developed the computer program that allows to recalculate the experimental phase diagrams into phase diagrams with given variables of the SAFV.

For water the coefficients values of SAFV for the first time were obtained for a complete set of 12 realizations of the SAFV. Herewith the experimental variables of the water CF were recalculated into the hypotetical variables of the Ising Model (IM), which led to rotation of the three-dimensional phase diagrams with respect to the CF three-dimensional diagrams. This rotation was carried out until the jump in the entropy vanishing along coexistence curve as it should be in case of IM. The verification showed within the limits of the experimental errors that with the entropy jump vanishing simultaneously the order field variable reached zero along coexistence curve as it should be also in case of IM. These and other tests showed that SAFV, largely similar to the Pokrovsky algebra [4,5], is correct for the description of CF experimental data. In contrast to the Pokrovsky algebra, this algebra takes into account the signs of the SAFV coefficients; and the values of parts of coefficients of SAFV are not small. Comprehensive analysis based on SAFV allowed to offer physical answers to questions 1-5. In particular, a new scaling criterion based on the scaling ideas of L.Kadanoff [8] has been proposed. With it the expansions of density and entropy in a series of thermodynamic derivatives have been written accounting of the asymmetric "2β" and non-asymptotic "1–2α" singularities (α=0,09±0,01 β=0,337±0,002 [9], then $1-2\alpha=\beta+\Delta$, Δ=0,48) for coexistence curve, as well as for case of critical isotherm, critical isochor, critical adabat etc. This type of corrections mathematically corresponds to the Van der Waals model of gas of fluctuations of the order parameter [1,10]. 12 forms of SAFV consistented with each other in combination with two small scale corrections gives complete quantitative description of CF in all fluctuation region within experimental errors. Based on experimental data for water, physical analysis within the SAFV leads to clear negative answers to questions 2-4. Physical meaning of the two-parameter renormalization operation can be suggested on the basis of Van der Waals model of gas of fluctuations of the order parameter [1,10], SAFV and law of corresponding states in accordance on ideas of K.Wilson.SAFV can be also rewritten for descriprion of spatially inhomogeneous CF under constant gravitational [1], electric and magnetic fields.

References

[1] A.D. Alekhin, *Izvestiya vuzov. Fizika* **4**, 39 (1983)
[2] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under Earth gravity, Politehnika, K: 2013.
[3] J. Wang., M.A. Anisimov, *Phys. Rev. E.* **75**, 051107 (2007).
[4] V.L. Pokrovsky *ZHETP Lett*, **17**, 4, 219 (1973).
[5] A.Z. Patashinskii, V.L. Pokrovskii Fluctuation Theory of Phase Transitions, Science, Moskow, 1982.
[6] W. Wagner, A. Pruss, *J. Phys. Chem. Ref. Data*, **31**, 2, 387 (2002)
[7] Ye.G. Rudnikov, A.D. Alekhin *Monitoring. Science and Technology* **3**, 89 (2013); **3**, 89 (2014); **3,** 59 (2015)
[8] L. Kadanoff *Physics* **2**, 263 (1966)
[9] A.D. Alekhin *Journal of Molecular Liquids* **120**, 43 (2005)
[10] A.D. Alekhin *Izvestiya vuzov. Fizika*. **3**, 103 (1983)

9-17.O

EVIDENCE FOR THE CONDENSATION IN THE DIVERGENCE REGION OF ACTIVITY EXPANSIONS

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Recent studies of Mayer's [1] cluster expansion (CE) have significantly advanced resolving a long-standing problem of modern physics – the statistical theory of the first-order phase transitions. A new generating function for the CE in terms of irreducible cluster integrals (virial coefficients) [2] has allowed derivation of equations that have a wider region of applicability in comparison to the conventional virial equation of state (VEoS). Those equations indicate the VEoS inadequacy (and actual constancy of pressure) beyond the point, ρ_G, where the VEoS isothermal bulk modulus vanishes.

The consequent studies of the CE in terms of reducible cluster integrals (i.e., the expansions for pressure and density in powers of activity, AVEoS) [3,4] have established the actual character of the AVEoS divergence exactly at the same ρ_G point: in fact, this divergence yields the density jump (beyond the ρ_G) at constant pressure and chemical potential (activity) that, in turn, corresponds to the first-order phase transition and confirms the results of the previous studies in terms of irreducible integrals.

The latest strict confirmation for the condensation phenomenon in the AVEoS divergence region has been obtained for the lattice-gas models. The "hole-particle" symmetry of such models directly indicates the equality of pressure (and chemical potential) at the saturation point, ρ_G, and boiling point, ρ_L, for the symmetrical equations of state in terms of both irreducible as well as reducible integrals. Moreover, the obtained general results exactly matches the well-known Lee – Yang solution [5] for a specific two-dimensional lattice-gas model.

References

[1] J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley, New York, 1977).
[2] M. V. Ushcats, Phys. Rev. Lett. **109**, 040601 (2012).
[3] M. V. Ushcats, L. A. Bulavin, V. M. Sysoev, S. Yu. Ushcats, Ukrainian Journal of Physics **62**, 533 (2017).
[4] M. V. Ushcats, L. A. Bulavin, V. M. Sysoev, S. Yu. Ushcats, Phys. Rev. E **96**, 062115 (2017).
[5] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).

9-18.O

BOILING TRANSITIONS ON TEXTURED SUPERHYDROPHOBIC SURFACES

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In this presentation I will discuss recent developments on the effect of texture superhydrophobic surface on the heat exchange and boiling phase transitions of liquid water phase in contact with a heated solid surface. The classical boiling curve for the heat exchange between a heated surface and a liquid pool features an initial phase of nucleate pool boiling during which the heat exchange is optimized, following by the film boiling phase, which is observed once the surface temperature is sufficiently high above the boiling point of the liquid, or what is known as Leidenfrost temperature. During the film boiling the liquid is fully separated from the solid surface by a stable vapor layer, which minimizes heat exchange and reduces the hydrodynamic drag between the solid and the liquid. Using high-speed camera imaging in a series of experiment in which heated metallic spheres are quenched in water we investigated the effect of surfaces wettability and texture on the film boiling transition. We found that on water repellent textured superhydrophobic surfaces the nucleate boiling can be fully suppressed, and film boiling observed at very low surfaces superheat [1]. The effect of the superhydrophobic surfaces vapor layer stabilization was later demonstrated to dramatically reduce the drag on heated metallic spheres falling in water [2] or to sustain a near zero drag sphere in gas cavity formation [3].

References

[1] I. U. Vakarelski, N. Patankar, J. Marston, D. Y. C. Chan, S. T. Thoroddsen, *Nature*, **489**, 274 – 277 (2012).
[2] I. U. Vakarelski, D. Y. C. Chan, S. T. Thoroddsen, *Soft Matter*, **10**, 5162-5169 (2014).
[3] I. U. Vakarelski, E. Klaseboer, A. Jetly, M. M. Mansoor, A. A. Aguirre-Pablo, D. Y. C. Chan and S. T. Thoroddsen, *Sci. Adv.*, **3**, e1701558 (2017).

SOLIDIFICATION LINE AND PROPERTIES OF LIQUID METHANE AT HIGH PRESSURES

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The methane solidification line is predicted using the canonical equations of state of the solid and liquid phases. Equations for Helmholtz free energy are written within the framework of thermodynamic perturbation theory, where the equations for the Helmholtz free energy of the Lennard-Jones fluid [1] and FCC crystal [2] appear as initial approximation, and the octupole-octupole interaction of methane molecules is taken into account as perturbation. The P-T dependence and densities of coexisting phases on the solidification line are calculated and compared to the existing experimental data. The thermodynamic properties of liquid methane are predicted over a wide temperature range (100-300 K) and pressures (up to 1GPa).

References

[1] J. Kolafa, I. Nezbeda, *Fluid Phase Equilib*. **100**, 1- 28 (1994).
[2] L. Yakub, *Int. J. Thermophys*. **35**, 1957- 1965 (2014)..

9-20.O

LOW-POWER OPTICAL IRRADIATION INFLUENCE ON ALCOHOLS DROPLETS EVAPORATION PROCESSES

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In the report the experimental data according alcohols (n-propanol, n-butanol, n-pentanol, n-heptanol, n-octanol and n-decanol) droplets evaporation into gas-vapor mixture of droplet substance's vapor and buffer gas under optical irradiation influence were considered. The experimental results were received for the nitrogen buffer gas pressure values 30, 50, 100, 200, 400 mm Hg and low-power (0,1 W) irradiation with wavelengths 390, 565 and 625 nm.
The measurements were carried out using the method, described in [1]. Experimental evaporation rate values were calculated from droplet's size dependence on time obtained by processing droplet's images. These images were received by using special camera, recording droplet in certain time interval. The droplets were hanged in working chamber at special suspension (chip transistor) allowing also to measure droplet's temperature with accuracy about 0,03 K. The values for the alcohols evaporation rate were calculated in the dark regime (without irradiation) as well as under the irradiation influence.
It wasn't obtained the irradiation influence at the rate of evaporation of low alcohols (1-propanol, 1-butanol, 1-pentanol). At the same time with the increasing of number of alcohol in homologous series the irradiation influence at the rate of evaporation is becoming more prominent. It was obtained the increasing of evaporation rate for the following alcohols: 1-heptanol (37%), 1-octanol (36%) and 1-decanol (85%) under the influence of irradiation with wavelength 390 nm for buffer gas pressure value 50 mm Hg. There is no n-heptanol droplets evaporation rate increasing under irradiation with other wavelengths λ=565 and λ=625 nm, while n-octanol and n-decanol evaporation rate increases even several times under irradiation with wavelengths λ= 625 nm (180% for decanol). It should be noted that radiation with λ =625 nm caused no change on the rate of evaporation for droplets benzene series (nitrobenzene, yodbenzene) and water [2].
By using experimental data it was shown that the temperatures of alcohol droplets under irradiation and in his absence virtually unchanged. Heating can't be the reason of a significant increase of the evaporation rate of irradiated droplets. This effect can be caused by the influence of exposure to collective movements in alcohol. Under the influence of surface radiation drops leaving no single molecule of alcohol but the whole group of molecules, which leads to a sharp increase in the rate of evaporation. All processes are listed in a drop of the surface layer as prepared previously given radiation absorption wavelengths showed no absorption in the bulk liquid for all investigated alcohols.

References

[1] G. M. Verbinska, A.V. Brytan, V.L. Karbovskiy, T.V. Kleshchonok, "Water and nitrobenzene droplets evaporation under ultraviolet irradiation", *Physics of aerodisperse systems*, **47**, 49-58 (2010) (in Ukrainian).
[2] A.V. Brytan, G.M. Verbinska, V.M. Sysoev, V.L. Karbovskiy, V.L. Cleshchonok, *Ukr. J. Phys*. **56**, 456-460 (2011).

9-1.P

STRUCTURAL AND PHASE TRASITIONS OF HYPEREUTECTIC SILUMINS PROCESSING BY PULSED ELECTRIC CURRENT IN LIQUID STATE

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Having a combination of low coefficient of thermal expansion, high specific strength and high wear resistance, hypereutectic Al-Si alloys are attractive for a range of applications such as liner-less engine blocks, cylinder liners, pistons and pumps. The properties of hypereutectic Al - Si alloys depend on the characteristics of cast microstructure and they can be improved by microstructure changes. The improvements in the mechanical properties, wear resistance are realized with the following changes: size, morphology (or shape), and distribution of primary and Si eutectic particles. Various methods can be employed to achieve previously mention improvements: the addition of some chemical elements such as Na, P, Sr, Ce. Alternatively, physical methods to the refinement of primary Si, including ultrasound, electromagnetic stirring and vibration, mechanical stirring have been attempted with limited success.

Over the past decade the Department of Physical-Technological Processes of Melting Aluminum Alloys, Physical and Technological Institute of Metals and Alloys of the NASU has developed the advanced technology in which a liquid alloy processing by pulsed electric current (PEC) with the periodic (cyclic) change of frequency. It has been shown that application of PEC prior to casting can lead to uniform refinement of solid solution grain structures and primary intermetallic phases.

In the present study, the effects of PEC on liquid hypereutectic Al - 18,5 % wt.Si alloy were studied in detail with differential thermal analysis, XRD and microscopy. It is shown that at the modes and methods of serve of electric signal worked out in-process the structure of fusion, near order of atoms, changes in the clusters of silicon, their size and by volume stake diminish. Hereupon the specific heat of crystallization of primary crystals of silicon diminishes more, than on 50 % and eutectic on 2 - 4 %, a temperature liquidus of alloy rises on 20 - 25 K and a solidus temperature goes down on 6 - 14 K as compared to descriptions of initial alloy. During crystallization a new modifications of silicon appear with the metallic type of inter-atomic interaction depending on the modes of electric-current pulse treatment. A size and amount of primary crystals of silicon diminish up to their complete absence in a microstructure at researches by the method of optical microscopy. The thinly differentiated of α-Al+β-Si eutectic is formed with the globular-like crystals of eutectic silicon.

9-2.P

EXTENDED EQUATIONS OF THE CRITICAL ISOTHERM AND THE GRAVITY EFFECT

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Based on the fluctuation theory of phase transition [1] and Van der Waals model of the fluctuations gas of the order parameter [2] of the system in the critical state, an extended equation of the state of substance has been investigated along the thermodynamic direction of the critical isotherm of a number of low- and high-temperature molecular liquids for homogeneous and inhomogeneous substances. For this purpose the P-V-T measurements data [3] and the gravity effect data [4] in an inhomogeneous system have been used. It has been shown that the amplitude of the asymptotic term of the critical isotherm equation of homogeneous system exceeds the corresponding amplitude of the equation of the gravity effect.
This result is explained in the paper by the appearance of the internal non-uniform critical field in the system under the action of the Earth's gravity field. It has been shown that molecular homogeneous liquids and inhomogeneous liquids in the Earth's gravity field are characterized by a diametrically opposite altitude asymmetry of the equation of state at the critical temperature. It has been shown that this result is related to the altitude asymmetry of the internal critical field [4] in inhomogeneous system. Physical meaning has been considered and comparative analysis has been carried out of the amplitudes of the equations both the critical isotherm and the gravity effect at the critical temperature of substance.

References

[1] A.Z. Patashinskii, V.L. Pokrovskii Fluctuation Theory of Phase Transitions, Science, Moskow, 1982.
[2] A.D. Alekhin Izvestiya vuzov. Fizika. 3. 103 (1983)
[3] https://webbook.nist.gov/chemistry/fluid/
[4] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.

9-3.P

MICRO-FLOATING METHOD OF HIGH-ALTITUDE DETERMINATION OF PRESSURE IN THE CRITICAL FLUID AND CONDITION OF ITS EQUILIBRIUM UNDER THE EARTH GRAVITY

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It has been provided a brief overview of the results of the experimental studies of the effect of gravity by optics techniques of light scattering and refractometry which indicating the nonlinear properties of an inhomogeneous critical fluid under the Earth gravity field [1]. The conclusion can be drawn that these properties of critical fluid are the basis of their practical use in modern industrial technologies [2].
A new experimental method of micro-floating manometer for high-altitude measurement of pressure in inhomogeneous critical fluid has been presented. It has been shown by using of the method that high-altitude change of pressure $\Delta P^*(z) = (P - P_c)/P_c$ in inhomogeneous critical fluid greatly exceeds the value of the hydrostatic pressure $|h| = \rho_c g|z|/P_c$ ($|\Delta P^*| >> |h|$). Based on this result and the results previously obtained by optical methods of light scattering and refractometry [3] the form of the condition of equilibrium $|\Delta P^*(T_c, L, \bar{\rho}| = (P - P_c)/P_c = |\Delta U^*(T_c, L, \bar{\rho}| = | >> |h|$ of inhomogeneous critical fluid under the Earth gravity has been confirmed. This equilibrium condition is dependent on the critical temperature, T_c, of substance, the linear size of the system, L, the average density of its filling by substance $\bar{\rho}$. This equilibrium condition is qualitatively different from the conditions of equilibrium $|\Delta P^*(z)| = |h|$ of inhomogeneous substance, proposed by van der Waals. T_c, P_c, ρ_c are the critical temperatures, pressure and density of substance.

References

[1] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.
[2] D.Yu. Zalepugin, N.A. Tilkunova, I.V. Chernyshova, et. al. Supercritical Fluids, 1 27 (2006).
[3] A.D. Alekhin, Journal of Molecular Liquids, 127, 1–3, 62 (2006).

THERMO RESPONSIVE HYBRID SYSTEMS DEXTRAN-graft-PNIPAM/EMBEDDED SILVER NANOPARTICLES

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The development of nano-sized materials that can perform a desired action upon a local or external stimulus is one of major goal of bionanotechnology. Thermoresponsibe responsible polymers based on poly(N-isopropylacrylamide) having conformational transition in the range of physiological temperature is discussed last years as novel drug delivery nanosystems. Star-like copolymer with dextran core and grafted poly(N-isopropylacrylamide) arms (D-g-PNIPAM) was synthesized, characterized and used as matrix for silver sols preparation. The comparative study of individual D-g-PNIPAM and nanohybrid system D-g-PNIPAM/embedded silver nanoparticles near lower critical solution temperature (LCST) has been done using Dynamic Light Scattering, UV-vis spectroscopy and Small angle X-Ray scattering. It was shown that the thermally induced collapse of end-grafted poly(N-isopropylacrylamide) chains above the LCST doesn't affect the size characteristics of silver nanoparticles in the hybrid nanosystem. It was shown that D-g-PNIPAM/AgNPs nanosystem contains 2 types of AgNPs: free nanoparticles which are formed outside of macromolecules and nanoparticles incorporated inside of polymer macromolecule. Obviously, these two types of AgNPs have various behavior in the region of conformational transition of polymer martix. Free nanoparticles remains free, but for incorporated silver nanopartcles the distance between them can change when polymer undergoes conformation transition.

References

[1] V. Chumachenko, N. Kutsevol, Yu. Harahuts, M. Rawiso, A. Marinin, L. Bulavin, J Mol Liq, **235**, 77-82(2017).

STUDY OF THE EFFECT OF OVERHEAT TEMPERATURE ON A STATE OF Pb-Sb ALLOYS

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It is known that at temperatures above the crystallization temperature in the melts of metals and alloys microconcentration heterogeneity is observed [1]. The phenomena occurred in the liquid state of metals and alloys are inherent in systems that are in critical state [2]. Such systems are characterized by a temperature, at which there are no complexes in the melt. The objective of this work was the investigation of the structural condition of Pb-Sb alloys, depending on the temperature of alloy heating above the liquidus curve, the cooling rate, as well as the determination of the boundary of a homogeneous and inhomogeneous state of the melt.

The investigations were performed for alloys with an antimony content of 5.0-20.0% (wt.), the rest is lead. The specimens were smelted in Taman's furnace with graphite heater at temperatures of 520-900 K and then heated by 50-250 K above the liquidus temperature and cooled with rates of 102 K/s, 103 K/s and 104 K/s. In the work we use differential thermal, metallographic, chemical and X-ray spectroscopic analyses.

In Pb-Sb alloys there are no changes in the phase composition occurred, irrespective of the heating temperature and the antimony content. Overheating of the melt above 170-250 K and aftercooling results in the formation of a fine-dispersed eutectic structure and suppression of the formation of primary crystals of lead and antimony compared with specimens with a lower overheating temperature.

The results of calculation with accounting for the first degree approximation of high-temperature expansion of the thermodynamic potential of binary alloy enable to obtain the curve of thermodynamic stability [3] for the melting of Pb-Sb alloys and make it possible to ascertain the temperature range, in which there were no microcomplexes in the melt, and also allow to predict the final structure of the alloy.

References

[1] L.A. Zhukova, S.I. Popel, *J. Phys. Chem.*, 56(11), pp. 2702–2706 (1982).
[2] E.V. Kalashnikov, *J. Tech. Phys.*, 67(4), pp. 7-12 (1997).
[3] O.M. Galdina, *Visn. Dnipr. Univ. Fiz. Radioel.*, 14(12/1), pp. 68-70 (2007).

SUPERCRITICAL PROPERTIES OF LIQUID AND MAGNETIC SYSTEMS

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According to classical theory of critical state in a critical point of a liquid system the liquid and the gaseous phases become identical, their physical properties becomes the same and above the critical point substance can exist only in a gaseous form. Numerous experiments indicate that supercritical area, remaining macroscopically homogeneous, becomes microheterogeneous within an interval of thermodynamic forces, which shows that above the critical point the property retention of subcritical phases occurs. From the point of view of thermodynamic stability [1] this indicates existence of a continuous supercritical transition between supercritical phases. It represents the system passing through a region of reduced stability, which leads to increase of fluctuations. The continuity of the transition is resulting from the fact that it occurs outside the instability area; there are neither jumps of thermodynamic coordinates, nor work and heat of transition. The region of great growth of energy fluctuations should not necessary coincides with the region of great increase of fluctuations of, for example, density. Therefore, curves of lowered stability for different stability coefficients need not be the same [2]. This confirms the fact that supercritical transitions take place in certain interval of thermodynamic forces.

For a magnetic system we have the same situation as for a liquid: under ferromagnetic transformation the system remains one-phase and transition represents it passing through a region of lowered stability, where mainly the structural transformation from one quasiphase to another takes place. Magnetic mesophase is a mixture of areas with different degrees of ordering of orbital and intrinsic moments. From the standpoint of thermodynamic stability ferromagnetic transformations are of the same mesophase nature as supercritical transitions in liquid-vapor system that shows macroscopically as similar run of the curves for stability determinant and coefficients [1].

The supercritical behavior of liquids and magnetics was studied by the example of several exactly-solved statistical models [3] and so-called classical models.

References

[1] E.D. Soldatova, *Cond. Matt. Phys.*, **2(4)**, pp. 603-616 (1999).
[2] O.M. Galdina, *Visn. Dnipr. Univ. Fiz. Radioel.*, **14**(12/1), pp. 68-70 (2007).
[3] E.D. Soldatova, O.M. Galdina, *J. Phys. Stud.*, **9**(4), pp. 325-332.

DISTINCTION AND SPEECH OF THERMAL HYSTERESIS WITH ITS ANALOGS

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Description magnetic hysteresis is useful in the analysis of thermal hysteresis by catalytic oxidation on the metal wire's surface of small impurities of combustible gases in air (Fig.1). The controlling parameter that affects the catalyst surface's temperature is environment's temperature T_g [1]. His choice is due to linear dependence on the wire's temperature in two basic regimes: low and high temperature.

Comparing two objects of temperature influence of heated wire: 1) air without combustible impurities and 2) ammonia-air and hydrogen-air mixtures. The first object behaves like a dia- or paramagnet with an increase-attenuation of the current, i.e. without temperature hysteresis. The hysteresis exists in the second object, but only in the region of sufficiently small impurity's concentrations Y_a. So, the stationary wire's temperature T characterizes the heated catalyst's surface, just like a magnetization in the domain structure of ferromagnets.

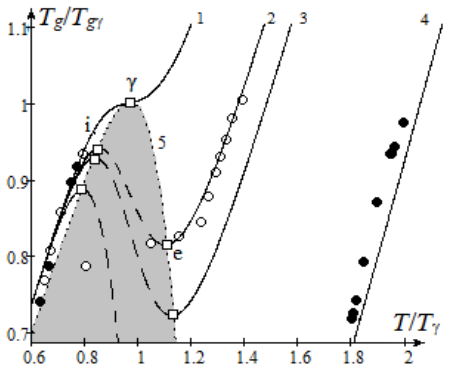

Fig. 1. Temperature of the hydrogen-air mixture depending on the stationary platinum wire's temperature [3] (diameter – 100 mkm, Sh = 0.5). Mass fraction of hydrogen in the air**:** 1) 0.05%, 2) 0.09%, 3) 0.108% 4) 0.19%. Curve 5 – spinodal. Parameters: T_{ov} = 408 K, T_v = 469 K.

The choice of the object of influence T and the control parameter T_g leads to the formal isomorphism of the heating-cooling curves in the coordinates $T(T_g)$ with a phase diagram of an equilibrium gas-liquid transition in a plane $\rho_{g,l}(p_{g,l})$. So there are matches: $T \leftrightarrow \rho_{g,l}$, $T_g \leftrightarrow p_{g,l}$, $Y_a \leftrightarrow T_{g,l}$, where the indices are g – gas, l – liquid). Thus, the impurity's concentration plays the role of temperature on the phase diagram (curves with a constant impurity's concentration look like isotherms when describing the phase transition of the gas-liquid).

Negative derivatives exist in coordinates $T(T_g)$: $\partial T / \partial T_g < 0$. But the second law of thermodynamics has no restrictions in this thermal hysteresis. The curve (spinodal) connecting the points i and e (points of catalytic self-ignition and extinction) describes critical value of the catalyst's initial temperature. High-temperature catalytic oxidation occurs with time when it is exceeded, and low temperature oxidation - when not heated.

References

[1] V.V. Kalinchak, A.S. Chernenko and V.V. Kalugin , *Journal of Engineering Physics and Thermophysics*. vol. 88, Iccue 3. P. 737-742 (2015).

UNIVERSALITY OF PERCOLATION PROCESSES IN POLYMER-CARBON NANOTUBES SYSTEMS

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In the framework of the critical percolation theory, the following scaling relations are used to describe the conductivity near the percolation transition point: $\sigma \propto (p - p_c)^t$ (1) for $p > p_c$, where σ is the conductivity of the system, p the filler concentration, p_c the critical filler concentration, and t are critical exponent for the electric conductivity. In the statistical percolation theory, the latter equal t ≈ 2 [1].

To analyze the influence of the features in the cluster formation and in the percolation cluster microstructure on the conductivity near the percolation transition point, we carried out the electrophysical researches of some oligoglycols and other polymers filled with multiwalled CNTs.

For neglecting of influence of microstructure factors on the behavior of the nanofilled polymeric systems near-by the percolation threshold we have found a scale function for conductivity. For the receipt of universal function of the percolating systems, we have normalized the eq. (1), dividing it into maximal conductivity after achievement of percolation threshold (σ_m) for the certain system and have passed to relative deviation from the percolation threshold [2]:

$$\frac{\sigma}{\sigma_m} = f\left(\frac{\varphi - \varphi_c}{\varphi_c}\right), \qquad (2)$$

where $f(x)$ is scaling function.

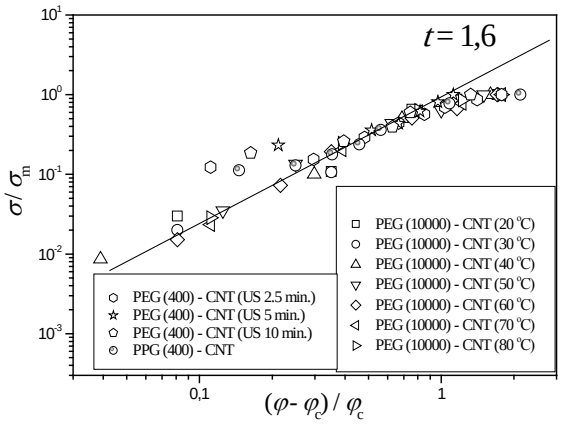

Fig. 1. Scaled dependence conductivity versus the relative concentration for polymer-carbon nanotubes systems.

We have applied this approach for the scaling of percolation curves for the polyether–CNT systems. Scale dependence in coordinates of the order parameter σ / σ_m and $(\varphi - \varphi_c)/\varphi_c$ for the polyether–CNT systems presented on fig. 1. From fig. 1 it is possible to see that in the narrow interval of approximation, what more small than φ_c, the experimental points of all of the probed dependences are almost imposed on one line, which corresponds the value of critical index of t = 1,6. Value of t = 1,6 is the universal value of critical index of conductivity, got by simulation on a three-dimensional resistor network and is very close to the vatue, got in the frame of Shklovskiy-de Genes model [3, 4]. From fig. 1 also evidently, that eq. (1) correctly describes experimental data only in narrow interval (to the critical area), which satisfies inequalities $(\varphi - \varphi_c)/\varphi_c < 1$. Deviation of experimental points from linearness in a concentration range $(\varphi - \varphi_c)/\varphi_c > 1$ is explained walking away from a critical area, where percolation curves can not be adequately described within the framework of scaling eq. (1). For the polyether–CNT systems concentration $(\varphi - \varphi_c)/\varphi_c \approx 1$ is a crossover – point in which the fluctuation behavior of conductivity changes on mean field (described by EMA).

Consequently, as an analysis within the framework of scaling approach shows, the probed systems show an universal percolation behavior regardless of as a polymeric matrix, methods of preparation and research conditions. The polyether–CNT systems can be attributed to one class of universality, and law (2), got for conductivity of the nanofilled systems analogical a law for other critical systems of class of universality of model of Ising (n = 1, d = 3), namely magnetics, individual liquids, binary low-molecular solutions and solutions of polymers with flexible chains.

References

[1] D. Stauffer, A. Aharony, Introduction to percolation theory (London: Taylor and Francis) 318 p. (1994).
[2] V.V. Klepko, E.A. Lysenkov, *Ukr. J. Phys.* **60 (9),** 944-949 (2015).
[3] A. Skal and B.I. Shklovskii, *Fiz. Tekh. Poluprov.* **8,** 1586 (1974).

TEMPERATURE AND COOLING RATE EFFECTS ON LUMINESCENT PROPERTIES AND PHASE STRUCTURE OF 5CB LIQUID CRYSTAL FILLED WITH CARBON NANOTUBES

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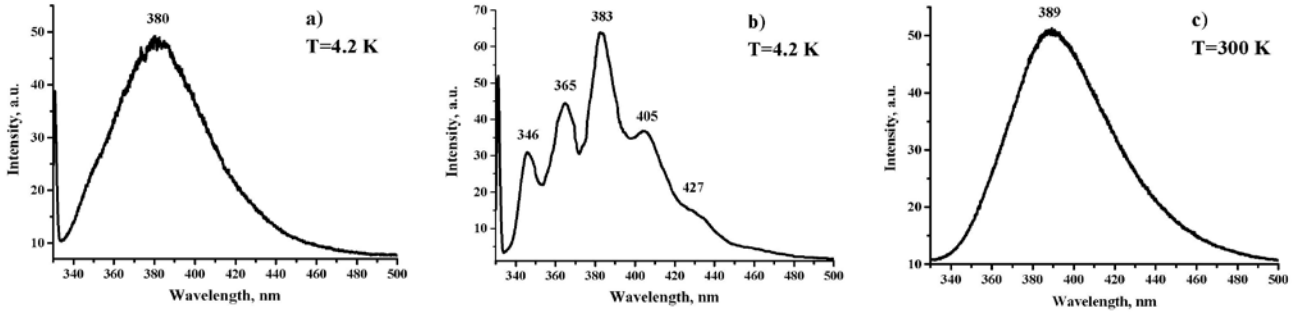
Liquid crystals (LC) 5CB (4-pentyl-4'-cyanobiphenyl) is a typical agent of cyanobiphenyl gomologous series with nematic phase existence interval of 297–309 K. Recently we have determined that the 5CB luminescence spectrum at T=4.2 K depends considerably on the sample cooling rates from the room to helium temperatures. Under slow (~2 K/min) cooling the luminescence maximum for pure 5CB shifts towards high wavelengths compared to fast cooling (~100 K/min). The results of differential scanning calorimetry experiments shows that the LC glassy state with glass transition temperature T_g=208 K is formed under the sample fast cooling regime. Luminescence of this phase is characterized by the structureless inhomogeneously broadened band with emission maximum at ~ 380 nm.

This work presents main results on the experimental investigations of the cooling rate effects on the luminescence properties and phase structure of the 5CB liquid crystal, doped with carbon nanotubes (NT). The figure shows luminescence spectra for the 5CB-NT samples under rapid (a) and slow (b) cooling, and also at the room temperature (c). The broad structureless radiation band at ~380 nm (a) is associated with glass-like state formation in the 5CB under rapid cooling of its isotropic phase down to T=4.2 K. Long-wavelength spectral shift (~9 nm) at T=300 K, compared to the spectrum at helium temperature is explained in the terms of conformational changes of the 5CB molecule, when a twisted conformation transfers gradually into a flat one with a subsequent formation of dimer structures. Slow cooling of 5CB-NT nanocomposite causes the fine structure in the LC luminescence spectrum (bands at 346, 365, 383, 405 nm), which appearance is discussed.



The correlation between the 5CB spectral luminescence properties and structure transformations has been established and analyzed for the 5CB-NT nanocomposites in a wide temperature range.

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9-10.P

PHASE TRANSITIONS INFLUENCE ON THE OXIDE STRUCTURES FORMATION ON THE SURFACE OF REFRACTORY METALS

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Oxides of refractory metals (e.g. tungsten, molybdenum) are widely used in sensor electronics and heterogeneous catalysis technologies. This fact causes a need to study methods of obtaining the refractory metals with specified characteristics. The aim of this work is to study an oxide film evaporation and the impact of melting on the process of forming branched oxide structures on the surface of refractory metal conductors heated by an electric current.
Temperature - time regimes of metal heating under which filamentary and lamellar crystals form on its surface have been studied. It has been proved that the crystals appear on the surface of a primary oxide layer in the places of its cracking. It has been determined that phase transitions such as melting of the oxide layer, evaporation and crystallization of oxide are significantly important in branching of the formed crystals. The growth rates of tungsten and molybdenum oxide crystals have been studied. It has been proved that at the beginning crystals grow more intensively in the longitudinal direction and then in the transverse direction [1]. The analysis of the obtained results enabled to determine the growth rate of crystals in different directions. It has been determined that the growth rates of tungsten oxide crystals are in the range $0.05 \div 0.3$ μm / s.
The fractal dimension has been determined in order to determine the model of crystal association at different stages of growth. It has been determined that at the initial stage association of crystals happens according to the "cluster-cluster" mechanism. Upon increasing growth time the "particle-cluster" mechanism is enabled. The growth rate of the crystals themselves also increases.

References

[1] S.G. Orlovskaya, M.S. Shkoropado, F.F. Karimova, *Physics and Chemistry of Solid State*, **14** (3), 527-531 (2013)

9-11.P

PECULIARITIES OF PHASE TRANSITIONS OF ALKANES

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Medium size alkanes (C18÷C35) are considered to be very promising materials for space utilization and energy storage applications. The melting behavior of alkanes is the decisive factor affecting their successful implementation. As it is known, the n-alkanes melting is a complex multi-stage process, which includes intermediate steps − recrystallization and pre-melting. To study the peculiarities of alkanes melting characteristics we used a method of suspended particle heating. The melting process of n-Octadecane (C18H38) and n-Docosane (C22H46) has been studied by videomicroscopy. The size and shape histories were obtained from the digital processing of the successive images of melting particles [1]. These curves were analyzed and compared with temperature dependencies of the alkane's physical properties (density, surface tension coefficient, refractive index). The melting times of particles of different sizes were determined at gas temperature slightly above the melting point (55÷60°C) and at relatively high temperature T_g =450°C, exceeding the boiling points of both alkanes. The phenomenon of surface freezing [2] was observed at alkane temperature above the melting point by 3÷4°C. The possibility was demonstrated to control the melting rate by dc electric field.

References

[1] F.F. Karimova, S.G. Orlovskaya, M.S. Shkoropado, *19th International Conference Digital Signal Processing*, **vol** II, 607-611 (2017).
[2] N. Maeda, *Phase transitions of long-chain n-alkanes at interfaces*. Lambert Academic Publishing. (2010).

9-12.P

ABOUT OPPORTUNITIES OF PRIME MOLECULAR MODEL AT THE SOLUTION OF PROBLEMS OF THERMODYNAMIC LEVEL

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The 145th anniversary of the famous Van der Waals equation of state (EoS) will be in 2018. For these years, the huge number of its empirical modifications was offered. However the quantity did not turn into quality. There is no efficient technique of the optimum EoS choice. The problem of creation of simple physically reasonable EoS is not solved.
We will begin the solution of the task with the analysis, systematization and searching of communication of the most prime models of two levels: molecular (objects and their interaction) and thermodynamic (EoS).
We allocate two molecular models – the point centers and spheres and two sets answering to them low-parametrical EoS. One - EoS of a vdw-type, which main lack - a loose coupling with microlevel. The second EoS group is received by the author on the basis of the interacting point centers (IPC) model [1]. All IPC EoS parameters make sense and are bound to manifestation of intermolecular forces. The operating parameters of two levels defining properties of model system, including a critical factor of compressibility of ZC are for the first time allocated and comprehended.
It is shown that many a vdw-type EoS can be included in a framework of new molecular- thermodynamic model. It is possible to establish their connection with microlevel and to receive answers to many questions [2]. The main part of them forms "a problem of the third parameter". The possibility of its decision is proved by the results obtained by us within a method of logical abduction.

References

[1]G.G.Petrik, Monitoring. Nauka i tehnologii, 1, 43-59 (2009).
[2] G.G.Petrik, Monitoring. Nauka i tehnologii, 3, 43-60 (2013).

9-13.P

MECHANISM OF VISCOUS FLOW OF ETHANOL AND 2,2,2-TRIFLUOROETHANOL

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Fluoroorganic compounds are widely used in practice. They have found their applications in nuclear power engineering and reactive technology, electronics, medicine, refrigeration and food industry [1].
Rheological properties of liquid ethanol-1 (C2H5OH) and 2,2,2-trifluoroethanol-1 (CF3CH2OH) were studied in the temperature range of 293-363 K. Density was measured by the pycnometric method, and the coefficient of kinematic viscosity was determined by the method of capillary viscometry.
For these liquids the density decreases linearly over the whole interval with increasing temperature, and the shear viscosity coefficient decreases exponentially. An analysis of experimental data indicates the dependence of density on the molecular mass of the liquid is similar for liquids with similar structure and type of intermolecular interaction. The replacement of hydrogen atoms by fluorine atoms in ethanol molecules results in increase of density and shear viscosity coefficient of the liquid.
The temperature dependence of the shear viscosity coefficient is well described by the Eyring equation [2]:

$$\eta_S = \frac{hN_A}{\chi V_\mu}\exp\left(\frac{\Delta H_\eta^{\neq}}{RT} - \frac{\Delta S_\eta^{\neq}}{R}\right),$$

where V_μ is the molar volume; h is the Planck's constant; N_A is the Avogadro's number; χ is the transmission coefficient, which represents the proportion of active complexes that overcome the potential barrier per unit time in the direction of shear force; $\Delta H_\eta^{\neq}$ and $\Delta S_\eta^{\neq}$ are changes of enthalpy and entropy of viscous flow; R is the gas constant. The relaxation time of the viscous flow is determined by the change in enthalpy in the transition of the molecule to the activated state. The replacement in ethanol of hydrogen atoms with fluorine atoms leads to growth of changes of enthalpy and entropy, relaxation time of viscous flow.

References

[1] P. Kirsch, Modern Fluoroorganic Chemistry: Synthesis, Reactivity, Applications, 320 (2004).
[2] Ya.I. Frenkel. Kinetic Theory of Liquids, 375 (1975).

EXACTLY THE SAME COMPLETE CANONIC FORMALISM OF THERMODYNAMICS AND CLASSICAL MECHANICS. APPLICATION FOR THE CRITICAL REGION

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Experimental investigations of the gravity effect by the method of molecular light scattering allowed to construct the scale function of the correlation length [1] and drew the attention to the importance of taking into account the field dependences [2] of physical quantities of the critical fluid. On this basis, the systematic method of thermodynamic potentials has been proposed [3]. Further development of this approach allowed us considering the equations of classical mechanics [4]. It has been shown for the first time that full canonic description of classical mechanics (Hamilton, Lagrange equations, equation for action $ds=p/N\cdot dq-H/N\cdot dt$ [3]) and thermodynamics can be presented using the same mathematical forms. The Fermat's principle of least action and the Second law of thermodynamics can also be written identically. A set of mechanic and thermodynamic relations have been obtained which mathematically coincide with Poisson brackets which notes the prospects for their using in quantum mechanics.

The full canonic formalism of classical mechanics (CFM) or thermodynamics (CFT) represents 240=48×5 equations in each case. Herewith diagram of thermodynamic square transforms to icosahendon diagram surrounded by hexahedrons and icosahendons, the same applies to the classical mechanics. It has been shown that equations for Hamiltonian $H/N(q,p/N)=H/N(1/q,r/N)$, momentum $p/N(t,H/N)=p/N(1/t,r/N)$, other variables always have dual forms that deepen the possibilities of conservation laws analysis:

$$d\frac{H}{N}=-\left(\frac{\partial\frac{p}{N}}{\partial t}\right)_{\frac{H}{N}}dq+\left(\frac{\partial q}{\partial t}\right)_{\frac{H}{N}}d\frac{p}{N}\qquad d\frac{H}{N}=-\left(\frac{\partial\frac{r}{N}}{\partial\frac{t}{q}}\right)_{\frac{H}{N}}d\frac{1}{q}+\left(\frac{\partial\frac{1}{q}}{\partial\frac{t}{q}}\right)_{\frac{H}{N}}d\frac{r}{N}\qquad \frac{r}{N}\equiv s-q\frac{p}{N}+t\frac{H}{N}$$

$$d\frac{p}{N}=-\left(\frac{\partial\frac{H}{N}}{\partial q}\right)_{\frac{p}{N}}dt+\left(\frac{\partial t}{\partial q}\right)_{\frac{p}{N}}d\frac{H}{N}\qquad d\frac{p}{N}=\left(\frac{\partial\frac{r}{N}}{\partial\frac{q}{t}}\right)_{\frac{p}{N}}d\frac{1}{t}-\left(\frac{\partial\frac{1}{t}}{\partial\frac{q}{t}}\right)_{\frac{p}{N}}d\frac{r}{N}\qquad (1)$$

It can be written for thermodynamics:

$$d\frac{S}{N}=-\left(\frac{\partial\frac{E}{N}}{\partial\frac{T}{P}}\right)_{\frac{S}{N}}d\frac{1}{P}+\left(\frac{\partial\frac{1}{P}}{\partial\frac{T}{P}}\right)_{\frac{S}{N}}d\frac{E}{N}\qquad d\frac{S}{N}=-\left(\frac{\partial\frac{V}{N}}{\partial T}\right)_{\frac{S}{N}}dP+\left(\frac{\partial P}{\partial T}\right)_{\frac{S}{N}}d\frac{V}{N}\qquad \mu\equiv\frac{E}{N}-T\frac{S}{N}+P\frac{V}{N}\qquad (2)$$

Lagrange equation and 47 mathematically equivalent equations for other classical-mechanics variables exactly match to 48 equations of thermodynamics.

The proposed based on CFT algorithm of the obtaining of thermodynamic inequalities for 48 main thermodynamic functions of state in the considered region of the phase diagram allows proposing an idea of extended-around Monte-Carlo method. Herewith the multy-probability concept has been introduced taking into account the imposition of inequalities conjuncted not only with entropy but also with other variables.

The proposed based on CFM 48 equations of Lagrange group equations allows expanding the scope of such numerical calculation algorithms as Werle schemes and proposing on this base an idea of extended-around Molecular Dynamic method. Herewith the multy-determinism concept has been introduced taking into account the sequential order of derivation for partial derivatives not only in time but also in other variables.

Exact mathematical match of CFT and CFM equations allows hoping that probabilistic and deterministic methods will be merged in the future.

In the critical region CFT and CFM was applied based on equilibrium P-V-T-data for example of water [5] using the developed computer program and on comparing of gravity effect data of equilibrium establishment for $T>T_c$ and $T<T_c$ [2], where T_c is the critical temperature.

References

[1] A.D. Alekhin ZhETP, 72, 5, 1880 (1972)
[2] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under Earth gravity, Politehnika, K: 2013.
[3] Ye.G. Rudnikov, A.D. Alekhin Monitoring. Science and Technology, 3, 74 (2013).
[4] L.D. Landau, E.M. Lifshitz Mechanics: Course of Theoretical Physics, Vol. 1 (1976)
[5] W. Wagner, A. Pruss, J. Phys. Chem. Ref. Data, 31, 2, 387 (2002)

9-15.P

ELECTRON SUBSYSTEM AS THE PRINCIPAL FACTOR OF PHASE TRANSITIONS

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When considered crystal-liquid phase transitions it's impossible not to take ignore the quantum nature of interatomic interactions. Here it's shown that the internal energy per one atom of ideal monatomic crystals (diamond, graphite, graphene, fullerene, nanotube, proteins) is of the form:

$$w(T) = -[U_S + U_A] + [V_S + V_A]\eta(T) + [W_S + W_A]\eta^2(T). \quad (1)$$

Here the factor $\eta(T)$ is the analog of the order parameter, but it has precise determination: $\eta(T) \equiv \left(1 + \exp\left(E_g / 2kT\right)\right)^{-1}$ where E_g is a forbidden band width ($0 \le \eta(T) < 1/2$, when $0 \le T < \infty$). Energies U_S, V_S and W_S consist only of centrally symmetric quantum-averaged energies of interaction between electrons with nuclei and with each other. In the far-field zone approximation, they have a Coulomb asymptotic behavior and are reduced to factors combination: $1/R$, where R is the distance between adjacent atoms. Energies U_A, V_A and W_A contains only centrally non-symmetric quantum-averaged energy of the exchange interaction. They select crystallographic directions and, in the far-field zone approximation they consist of factors combination: $\varphi_f(-\mathbf{R})\varphi_g(\mathbf{R})/R$. Factors $\varphi_f(\mathbf{R})$, $\varphi_g(\mathbf{R})$ are wave functions for the valence band $(\{f,g\} = v)$ or the conduction band $(\{f,g\} = c)$. For condensates of the carbon series in (1) for crystallographic directions, always the condition is satisfied: $U_S + U_A > 0$. That is, at zero temperature ($\eta = 0$) the energy (1) is negative (corresponds to the bound state). Also, in this case, the condition $W_S + W_A > 0$ is always met. That is with the temperature rise this summand uniquely provides an increase in energy. The factor $V_S + V_A$ can be positive or negative. But this factor is small and has no effect on the general tendency of increasing energy with the temperature rise.

It is shown that the condition: $-U_A + V_A\eta(T) + W_A\eta^2(T) = 0$, determines the temperature value for the crystal-liquid phase transition, since it is associated with the absence of anisotropic contributions to the interatomic interactions. And the condition: $-U_S + V_S\eta(T) + W_S\eta^2(T) = 0$, determines the point of the liquid-gas transition, because it eliminates the rest of centrally symmetric short-range interatomic interactions.

9-16.P

THE JOULE-THOMSON EFFECT IN A CRITICAL FLUID IN THE EARTH'S GRAVITATIONAL FIELD

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It has been examined the Joule-Thompson effect on the mechanical equivalent of heat in a critical state of matter. The experimental data of the gravitational effect obtained by optical light scattering and refractometry [1] in the critical state of the substance are analyzed for this. In the transition of such an inhomogeneous system to a homogeneous but non-equilibrium state, the critical temperature of the substance decreases from T_{c1} K $T_{c2} < T_{c1}$, [2,3].
The decrease in T_{c2} of homogeneous systems is associated with the expenditure of the energy of fluctuations of the order parameter [4] of the inhomogeneous system $\Delta F_f/(P_c V_c) = \int_L C_0 R_c^{-3}(T_{c1}, \Delta\mu(\mathrm{h})\mathrm{dh})$ when the center of mass of a non-equilibrium homogeneous system moves by a distance z in an optical cell of height L. The change in thermal energy in this non-equilibrium state of the substance [4] is represented in the form: $\Delta Q = d^2F_f/dt^2 \cdot t = C_v \cdot t = C_0 \cdot r_0^{-3} \cdot 3\nu \cdot (3\nu - 1) \cdot t^{1-\alpha}$.
The calculations of ΔF_f and ΔQ in [5] for n-pentane at $t = (T_{c1} - T_{c2})/T_{c1} \approx 10^{-3}$ indicate that their values are close in the presence of an inhomogeneous internal field in an inhomogeneous system, $\Delta\mu(h) = d\mu/dh \cdot h \approx 10^2 h >> h = \rho_c g z/P_c$.
Thus, the obtained result indicates the validity of the Joule-Thompson effect: the mechanical equivalent of heat, or the thermal equivalent of the work for inhomogeneous fluctuation systems in the critical state of matter.

References

[1] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.
[2] A. Polt, B. Platzer, G. Maurer, Chem Tech., Leipzing, 44, 6, 216 (1992)
[3] L.A. Bulavin Properties of liquids in the critical region, Kyiv University, 2002
[4] A.Z. Patashinskii, V.L. Pokrovskii Fluctuation Theory of Phase Transitions, Science, Moskow, 1982.
[5] A.D. Alekhin, Ukrainian Journal of Physics, 33, 1, 152 (1988).

9-17.P

THERMODYNAMIC RESPONSES OF ANY ORDER FOR WATER IN THE FLUCTUATION VICINITY OF THE CRITICAL POINT

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Until now, there has been no reliable method for calculating the pair correlation function that quantitatively corresponds to the experimental behavior of a condensed substance with an asymmetric equation of state near the critical point. For correlation functions of the third order and higher orders, even obtaining general forms of correlation functions is considered to be an unsolved problem [1].

With using of Kadanov's ideas [2] the sequential chain method of calculation of thermodynamic responses nearby to the critical point has been proposed for the first time. This method is based on the proposed complete canonical formalism of thermodynamics and symmetric algebra of the fluctuation variables (SAFV) [3]. Wherein the quantitative confirmation of the SAFV has been obtained using the experimental P-V-T-C_v-β_T-β_S data for water [4] within experimental errors in the fluctuation vicinity of the critical point.

Taking into account the peculiarities of the experimental behavior of the thermodynamic coefficients in the super-critical and sub-critical region, exact solutions of SAFV for thermodynamic responses of any order have been obtained. This allows writing the expressions for the correlation functions of any order for any field and density variables for all close region near the critical point. Coefficients of ordered and unordered contributions [3] to the correlation function can be determined from the experimental data [4]. The scaling representation forms of the SAFV mathematically correspond to Van der Waals model of the fluctuation gas [5,6] of the order parameter with coefficients having physical meaning.

References

[1] A.Z. Patashinskii, V.L. Pokrovskii Fluctuation Theory of Phase Transitions, Science, Moskow, 1982.
[2] L. Kadanoff Physics 2, 263 (1966)
[3] Ye.G. Rudnikov, A.D. Alekhin Monitoring. Science and Technology, 3, 59 (2015).
[4] W. Wagner, A. Pruss, J. Phys. Chem. Ref. Data, 31, 2, 387 (2002)
[5] A.D. Alekhin Izvestiya vuzov. Fizika. 3. 103 (1983)
[6] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.

9-18.P

COUPLING OF SHEAR VISCOSITY, DIFFUSION AND THERMAL CONDUCTIVITY COEFFICIENTS IN THE CRITICAL REGION: THEORY AND EXPERIMENT

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Theory.

For the simplest case of the liquid-vapor critical point the scaling interconnections among coefficients of shear viscosity, diffusion and thermal conductivity have been proposed. Wherein instead of diffusion coefficient D in Fick's equation $d(N/V)/d\theta=-D\cdot dx/dz$ the coefficient $D^{/}$ in the modified Fick's equation $d(N/V)/d\theta=-D^{/}\cdot d\mu/dz$ was used. Then it will be satisfied in the neighborhood of the critical point the condition $D^{/}\sim R_c$, since $d\mu/dx\sim R_c^{-\gamma/\nu}$ [1] and $D\sim t^{\gamma-\nu}\sim R_c^{-1+\eta}$ [1] (R_c is correlation length of long-scale fluctuations of the order parameter). This means that the scaling behavior of modified diffusion coefficient $D^{/}$ and thermal conductivity coefficient κ ($d(E/N)/d\theta=-\kappa\cdot dT/dz$ or $d(S/N)/d\theta=-(\kappa/T)\cdot dT/dz$) will be qualitatively the same: ($\kappa\sim t^{-\nu}\sim R_c$ [1]). To include the shear viscosity coefficient η in a unified analysis scheme using the scaling approach [2], it was shown that scaling behavior of momentum flux $d(p/N)/d\theta$ and of specific volume flux $d(V/N)/d\theta$ is also qualitatively the same. On this basis Newton's equation $d(p/N)/d\theta=-\eta\cdot dv/dz$ was rewritten in the modified form $d(V/N)/d\theta=-\eta\cdot const\cdot dP/dz$. The relationship of the pressure gradient in this modified Newton's equation with the temperature gradient (Fourier equation) and chemical potential equation (modified Fick's equation) is established using the Gibbs-Duhem equation. Therefore, the scaling behavior of shear viscosity, diffusion and thermal conductivity coefficients should be qualitatively the same ($\eta\sim D^{/}\sim\kappa\sim t^{-\nu}\sim R_c$). But this conclusion contradicts the conclusion from the Dynamic Scaling theory for shear viscosity coefficient ($\eta\sim R_c^{Z\eta}$, Z_η=0,06) [1,3].

Experiment.

It was necessary to check which conclusion is correct: $\eta\sim R_c$ (the conclusion made above) or $\eta\sim R_c^{z}$ (Dynamic Scaling [3]). Analysis of complex experimental investigations of concentration and temperature dependences of the shear viscosity of the solution [4] has been shown that along the thermodynamic direction of the critical iso-concentrate, these two cases are indistinguishable. At the same time, an analysis of the thermodynamic directions of the critical isotherm and the coexistence curve leads to the definite conclusion that $\eta\sim R_c$. This behavior of the shear viscosity confirms with the formula for the critical viscosity with accounting the system spatial dispersion proposed by A.D. Alekhin [5]. Using of this formula [5] led to the conclusion that concentration and temperature dependences of the fluctuation part of the shear viscosity $\eta\,(x,T)$ for a molecular solution of isobutyric acid-water are quantitatively described by the formula of critical viscosity [5] within the limits of experimental errors with constant wave vector $q=0,02\pm0,002$. Estimates show that the role of spatial dispersion increases with the transition to metal melts [6], in this case $q\approx0,1$. The presence of dispersion [5] can be explained by the fact that the liquid flowing through the capillary of the viscometer is non-equilibrium. It is concluded that the theory of dynamic scaling should be used to describe acoustic data near the critical point.

An analysis of the shear viscosity behavior $\eta\sim R_c$ on the basis of formula of critical viscosity [5] in accordance with the modified Newton formula shows failure of expression “critical slow down” since it follows from viscometry experimental data that as the pressure gradient increases, the volume flow increases. It is suggested that this expression be replaced by an expression of the opposite meaning “critical activization”. Coefficients of shear viscosity, diffusion and thermal conductivity strongly increase as the critical point is approached ($\eta\sim D^{/}\sim k\sim R_c$), since the heat, mass, momentum, internal energy, and volume transfer is improved (but not degraded) by large-scale fluctuations of the order parameter, and the viscous friction force increases. Proposed physical interpretation of this phenomenon is essentially new.

References

[1] M.A. Anisimov Critical phenomena in liquids and liquid crystals, Philadelphia: Gordon and Breach, 1991.
[2] L. Kadanoff Physics 2, 263 (1966)
[3] L. Kadanoff Phys. Rev. 1, 89 (1968)
[4] A.D. Alekhin, Ye.G. Rudnikov, Yu.L. Ostapchuk, Monitoring. Science and Technology 1, 52 (2015)
[5] A.D. Alekhin , Ukrainian Journal of Physics 2, 138 (2004).
[6] L.A. Bulavin, Yu.O. Plevachuk, V.M. Sklyarchuk. Critical phenomena of exfoliation in liquids on Earth and in space, Kyiv, Naukova Dumka (2011).

9-19.P

FIELD ASYMMETRY OF THE GRAVITY EFFECT AND INHOMOGENEOUS FIELD IN INHOMOGENEOUS CRITICAL FLUID

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A brief review of the results of studies of the gravity effect in the critical fluid (CF) [1] namely inhomogeneous of substance under the critical state has been presented in the paper based on the data of light scattering, refractometry, and slow neutron passing methods. On the basis of these data, the field-altitude asymmetry of various properties of an inhomogeneous substances has been analyzed: the order parameter $\Delta\rho(z)$ ($|\Delta\rho(h>0,z>0, \rho<\rho_K)|>|\Delta\rho(h<0,z<0,\rho>\rho_K)|$), the density gradient $d\rho(z)/dz$ of the substance ($|d\rho/dh(h>0,z>0,\rho<\rho_K)|>|d\rho/dh(h<0,z<0,\rho>\rho_K)|$), the intensity of the scattered light I(z) ($|I(h>0,z>0,\rho<\rho_K)|<|I(h<0,z<0,\rho>\rho_K)|$). It has been shown [2] that the sign of the altitude asymmetry of these equilibrium properties of an inhomogeneous substance is related to their kinetic characteristics: the diffusion coefficient D(h) ($|D(h>0,z>0,\rho<\rho_K)|>|D(h<0,z<0,\rho>\rho_K)|$) and the viscosity coefficient η(h) ($|\eta(h>0,z>0,\rho<\rho_K)|<|\eta(h<0,z<0,\rho>\rho_K)|$) when the system transforms from a homogeneous state to an inhomogeneous state under (z) $|\mu$ the action of an internal asymmetric field $|\Delta U(z)|= |\Delta\mu(z)|>>|h=\rho_C gz/P_C|$ (z is the height read the meter from the level with critical density of substance). According to the gravity effect [1] and P-V-T [3] data, the magnitude of the altitude variation of this field and its dependence on the critical temperature of the substance has been found.

References

[1] A.D. Alekhin, A.K. Dorosh, Ye.G. Rudnikov Critical state of substance under the Earth gravity, Politehnika, Kiev, 2013.
[2] A.D. Alekhin, Monitoring. Science and Technology, 1 (2018).
[3] https://webbook.nist.gov/chemistry/fluid/

ALCOHOL'S DROPLETS EVAPORATION FOR THE TRANSIENT EVAPORATION REGIME

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Investigation of the kinetics of organic liquids droplet's evaporation, including alcohol, is the actual practical problem associated with modeling the behavior of particular biofuels in combustion chamber [1]. In theoretical studies it was shown that the evaporation of liquid droplets in the surrounding gas atmosphere at pressures lower than atmospheric mass transfer process ceases to be diffusion. The criterion for rejection is the Knudsen's number $Kn=\lambda/r$: ratio of the mean free path of the molecules of matter drops to its range

This work is devoted the consideration of the experimental dependence of the evaporation's rate of substances homologous series of alcohols (n-propanol, n-butanol, n-pentanol, n-heptanol , n-octanol) on buffer gas various pressure's value. Experimental evaporation rate values were calculated from droplet's size dependence on time, which was obtained by processing droplet's images. These images were received by using special camera, recording droplet in certain time interval. The droplets were hanged in working chamber at special suspension (chip transistor) allowing also to measure droplet's temperature with accuracy about 0,03 C^o.

The experimental dependence of the rate of evaporation of inverse pressure were analyzed using the theory of evaporation Fuchs [2]. It has been shown that the deviation from the diffusion regime of evaporation becomes significant for the pressure less than 100 mmHg. century. Calculated values of Knudsen numbers that meet the conditions of the experiment. It is shown that the deviation from the diffusion regime of evaporation for droplets with an average radius of 0,09 cm, it is essential for the Knudsen number order 10^{-3}. It was calculated evaporation coefficient's values by using theoretical expression, which describe evaporation in transient regime of evaporation.

References

[1] O. Samimi Abianeh, C.P. Chen, International Journal of Heat and Mass Transfer, 55, 6897–6907 (2012).
[2] N. A. Fuchs, A. G. Sutugin. Highly Dispersed Aerosols.– Michigan : Ann Arbor Science Pubisher, Ann Arbor, 1970. – 105 p.

Section 11. Nonextensive Thermodynamics of Liquid Systems

Oral session

11-1.O

MICROSCOPIC STUDY OF SOLID/LIQUID INTERFACES WITH MOLECULAR DYNAMICS

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The interfaces between liquids and solids predominate a variety of physical and chemical properties, especially at the nanoscale, where the surface-to-volume fraction becomes larger. Experimental studies are difficult and they need to be calibrated at the nanoscale, so prediction of the physical and chemical properties with atomistic simulations to obtain answers for a variety of applications like energy, chemical industry, catalysis engineering, material science, microfluidics, pharmacology, medicine, etc.
In this report the silicon-water interfaces are studied with means of molecular dynamics simulations. Lennard-Jones potential is applied for the interaction between water molecules and silicon atoms, while interactions between silicon atoms are performed with Tersoff interatomic potential. First we evaluated the epsilon parameter of the Lennard-Jones potential and our methodology can be applied in difference systems with the simple knowledge of the experimental macroscopic contact angle. Furthermore the adsorption layer of water molecules is estimated and the importance of this layer for nanoscale droplets is analyzed.

11-2.O

STABILITY OF SHEAR-THINNING FLUID IN OPEN-CHANNEL

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The Orr-Sommerfeld equation governs the stability of a 2D laminar parallel flow in the x-direction for a Newtonian flow of stationnary velocity $\overline{U}$ and Reynolds number Re submitted to infinitesimal 2D perturbations of celerity c and wave number k in the (x-y) plane. Denoting the disturbance stream function by ψ, it writes [1]:

$$\left(\overline{U}-c\right)\left(\partial_{yy}-k^2\right)\psi-\partial_{yy}\overline{U}\psi=\frac{1}{ik\,\mathrm{Re}}\left(\partial_{yy}-k^2\right)^2\psi \qquad (1)$$

The occurrence of roll waves at the surface of a liquid layer is of major importance in process engineering as they would produce a non-uniform matter deposition in coating application. Polymer fluid follows a shear thinning rheological behaviour [2]. It is generally described by the power-law rheological equation [3] which makes it possible to represent decreasing in viscosity as shear increases. The method of integral relations was used with power-law equation in [4] to derive an evolution equation for two types of waves, say dynamic and kinematic waves and in this way, are difficult to exploit as they cannot be easily compared to the Newtonian case.
In this paper, a rigorous model of stability of power-law fluid over an incline, based on the statement and resolution of an Orr-Sommerfeld equation generalized for power-law fluid in order to compute the effect of fluid rheology and flow control parameters on flow stability.

References

[1] Orr, W.M. (1907): The stability or instability of the steady motions of a perfect liquid and of a viscous liquid., Proc. R. Irish Acad A., 27:9-68, 69-138.
[2] Bird, R.B., Armstrong, R.C. & Hassager, O. (1987): "Dynamics of polymeric fluids (Fluid Dynamics I)", Wiley, New York
[3] Nsom, B., Ravelo, B. & Ndong, W. (2008): Flow regimes in viscous horizontal dam-break flow of clayous mud. Appl. Rheol., 18(4), 43577-1 – 43577-8
[4] Dandapat, B.S. & Mukhopadhyay (2001): Waves on a film of power-law fluid flowing down an inclined plane at moderate Reynolds number. Fluid Dyn. Res., 29, 199-220

MOLECULAR SIMULATIONS OF SURFACTANT ADSORPTION AND SELF-ASSEMBLY UNDER STATIC AND SHEAR CONDITIONS

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Lubricant additives are essential in the automotive industry to ensure the smooth operation of modern engines by reducing friction, wear, oxidation, and corrosion, as well as providing thermal stability and removing debris. Many additives are organic and amphiphilic, which means that they can form aggregates in aqueous and non-aqueous solvents. In this work, large-scale atomistic molecular dynamics simulations are used to study the competition between adsorption and self-assembly in solutions of typical additives under strong confinement between inorganic surfaces, under both static and shear conditions. It is found that in non-aqueous solvents under static conditions, lubricant additives (an organic friction modifier and a polymeric soot dispersant) and their mixtures can form stable reverse micelles for a range of concentrations. With the application of shear, the reverse micelles disintegrate and the additive molecules partially adsorb on to the surfaces. Friction is studied in the sheared systems, and it is observed that friction is minimised in a binary mixture of the additives. It is found that friction reduction is directly connected with the existence of aggregates. In aqueous solutions of cetyltrimethylammonium bromide (CTAB) confined between mica surfaces, it is found that CTAB forms lamellar structures on the surfaces, as a result of the slow solvation of the mica K^+ ions in water. The CTAB simulations shed light on a range of recent experimental measurements [1] and reveal the molecular-scale mechanism of bilayer formation.

References

[1] L. R. Griffin, K. L. Browning, C. L. Truscott, L. A. Clifton, and S. M. Clarke, *J. Phys. Chem. B* **119**, 6457-6461 (2015).

MOLECULAR MODELLING ON 1-1`-SPIROBIPIRROLIDINIUM TETRAFLUOROBORATE ACETONITRILE SOLUTIONS IN MULTI-WALLED CARBON NANOTUBES

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Multi-walled carbon nanotube (MWCNT) is a cylindrical nanoscale object formed by multiple atomic layer of carbon atoms. It was demonstrated that carbon nanotubes can be used as materials for constructing electric double-layer capacitors (EDLC) due to a high degree of structure symmetry and great surface inside [1].
Acetonitrile solution of 1-1`-spiropyrrolidinium tetrafluoroborate ($SBPBF_4$/AN) shows higher conductivity as compared with analogs [2], therefore it was chosen as electrolyte solution for investigated systems.
In present work the influence of spatial confinements caused by internal space of MWCNT on microscopic structure and particle dynamics of concentrated $SBPBF_4$/AN solution is investigated by means molecular dynamics simulation (MD).
Classical MD simulations were carried out using GROMACS program package. All molecules and ions were treated within the full atom approach. Rigid infinite MWCNT was fixed inside rectangular prism simulation box (fig. 1).

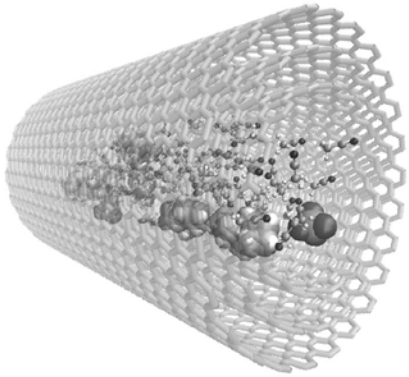

Figure 1. Snapshot of the 1M $SBPBF_4$/AN solution inside of MWCNT ((15,15),(20,20),(25,25)).

The results of our analysis have shown that MWCNT greatly influence on the structure and particle dynamics of $SBPBF_4$/AN solutions.

References

[1] P. Sharma and T.S. Bhatti, *Energy Convers. Manag.*, **51**, 2901–2912 (2010).
[2] N. Jackson and M. Payne, *ECS Trans.*, **16**, 139-149 (2008).

11-5.O

SURFACE TENSION IN BULK AND CONFINED LIQUIDS

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This presentation is aimed at theoretical studies the surface tension coefficient and its relation to the available experimental data. The following problems are going to be discussed: 1. The surface tension and capillary constant in bulk and spatially bounded liquids in a wide range of thermodynamic parameters (temperature, density, pressure), including the critical region. 2. The influence of size effects on the coefficient of surface tension and the capillary constant in liquids with a varying spatial dimensionality from the "bulk" state to the "surface" (two-dimensional) state. Here, we shall study the dimensional crossover of two types: 1) as transition from 3d bulk liquids to 3d bounded liquids, 2) as a smooth change in linear dimensions from the "bulk" state to the "surface" (two-dimensional) state. 3. The fluctuation effects are studied at 2d-3d-4d dimensional crossover for confined liquids with different lower crossover dimensionality. 4. The application of the obtained results to the problem of nucleation of a new phase with the isomorphism hypothesis between processes of nucleation and carcinogenesis taken into account.

References

[1] B.Widom, J. Chem. Phys. 43, 3892-3897, 1965
[2] V.N.Grigor'ev, N.S.Rudenko, Sov. Phys. JETP **20**, 63, 1965.
[3] Yu.P. Blagoi, V.V.Pashkov Sov. Phys. JETP **22**, 999, 1966.
[4] J.S. Rowlinson, B.Widom, Molecular Theory of Capillarity, Clarendon Press, Oxford, 1982.
[5] V.G.Baidakov et al. Preprint Ural Scientific Center Acad Sci USSR, Sverdlovsk, 1983.
[6] A.V.Chalyi. Proc. All-Union Symposium on Physics of Solid State Surfaces, ed. A.N.Naumovets, Kiev, 1983.
[7] A.V.Chalyi, Rep. Natl. Acad. Sci. Ukraine **9**, 170, 2012
[8] L.A.Bulavin, A.V.Chalyi, Modern Problems of Molecular Physics, Springer Proceedings in Physics, **197**, 253, 2018.

11-6.O

WATER IN INTERLAYERS AND MICROPORES IN HARDENED CEMENT PASTES

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Among materials with micro- and mesopores hardened cement paste is of outstanding technical importance. Its drying, shrinkage, and swelling due to variation of the relative humidity are very important for durability, resilience, and the structural design of concrete members. At low humidity, condensed water is already present in micropores and as interlayer water within the C-S-H phase. In several types of concrete compositions, pronounced hysteresis of water vapor sorption and volume change of the solid structure at low humidity is frequently observed.
We developed a theoretical model that can explain water-vapor sorption hysteresis and its connection to hysteresis of swelling and shrinkage based on water sorption in micropores and interlayer water [1-3]. The condensed water can exert capillary forces that change the volume of pores, which are embedded in elastic solids. Using computer simulations, we have studied the impact of chemical details of slit-pore walls of different cement pastes on thermodynamic and structural properties of condensed water.

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References

[1] P. Schiller, M. Wahab, T. Bier, S. Waida, H.-J. Mögel, *Procedia Materials Science*, **11**, 649-654 (2015).
[2] P. Schiller, M. Wahab, T. Bier, S. Waida, H.-J. Mögel, *Journal of Materials Science and Chemical Engineering*, **4**, 40-48 (2016).
[3] P. Schiller, M. Wahab, S. Waida, T. Bier, H.-J. Mögel, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **513**, 76-86 (2017).

11-7.O

MOLECULAR SIMULATIONS OF FUNCTIONALISED COPOLYMERS IN BULK AND IN CONFINEMENT: UNCOVERING THE ROLE OF FUNCTIONAL-GROUP DISTRIBUTION

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Organic additives in oil-based lubricants are used to reduce friction, reduce wear, reduce oxidation, increase performance, improve viscosity index, and even control the way the oil degrades. With such important roles being played by the additives, it is imperative that the physical mechanisms of action are understood, so that better, more efficient lubricants can be developed. This work is focused on atomistic molecular dynamics (MD) simulations of polymeric additives possessing different distributions of polar functional groups (FGs) attached to a polyethylene-polypropylene copolymer backbone.
The functionalised copolymers are immersed in a non-polar solvent, either in bulk or in confinement between parallel iron-oxide walls. The MD simulations reveal that the size of the copolymer – as measured by the radius of gyration R_g or the end to end distance R_{ee} – is very sensitive to the distribution of FGs on the backbone. This is shown to be due to the association of the FGs, and the detailed atomistic interactions responsible for this are elucidated. In addition, predictions of the form factor, $P(q)$, can be tested against results from small-angle neutron scattering experiments. Similarly, MD simulations of confined copolymer solutions point towards a link between the functional-group distribution and the adsorption of the copolymers on to the iron-oxide surfaces, particularly the copolymer's lateral spread and normal height, measured through R_g and mass-density profiles. Some links between these structural properties and the tribological effects of functionalised copolymers are put forward [1].

References

[1] R. F. G. Apóstolo, P. J. Camp, B. N. Cattoz, P. J. Dowding, and A. D. Schwarz, *Mol. Phys.*, (submitted).

11-8.O

EFFECTS OF DIMENSIONALITY CROSSOVER ON LIGHT AND NEUTRON SCATTERING IN LIQUIDS AT RESTRICTED GEOMETRY

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This presentation is aimed at studying the influence of dimensionality, or dimensional, crossover (DC) on spectra of the light molecular scattering (LMS) and quasi-elastic neutron scattering (QENS) and its possible medical applications. Specific characteristics of LMS and QENS spectra in confined liquids were studied with taking effects of DC from 3D to 2D systems into account. The transition between 3D and 2D behavior of LMC and QENS parameters were found in their dependence on size, temperature, pressure, and density variables. It was shown that decreasing the system's size L (e.g. the thickness of liquid films, slitlike pores, biological membranes, synaptic clefts, etc.) causes such changes in spectra of LMS and QENS : 1) the width Γ_c of the central Rayleigh line and the width $\Delta E(q^2)$ of the QENS peak, are rapidly increasing because $\Gamma_c \sim \Delta E(q^2) \sim L^{-2}$; 2) the width Γ_{MB} of the Mandelstam-Brillouin components in LMS spectra is strongly shortening, being proportional L^3; 3) the frequency shift $\Delta\Omega_{MB}$ of the Mandelstam-Brillouin components is weakly increasing according to $\Delta\Omega_{MB} \sim L^{-0,087}$; 4) the Landau-Placzek relation is essentially decreasing in accordance with $I_c/2I_{MB} \sim L^{1,79}$. These results give a precise diagnostic method of the cell proliferation (growth of cell and membrane sizes) for detecting the process of tumor formation.

References

[1]. K.A. Chalyy, K. Hamano, A.V.Chalyi, J. Mol. Liquids **92**, 153, 2001.
[2]. K.A. Chalyy, L.A. Bulavin, A.V.Chalyi, J. Phys. Studies **9**, 66, 2005.
[3]. L.A. Bulavin, K.A. Chalyy, Neutron Optics of Mesoscale Liquids - K.: Naukova Dumka, 2006.
[4]. F.M. Gasparini, M.O. Kimbell, K.P. Mooney, M. Diaz-Avila, Rev. Mod. Phys. **80**, 1009, 2008.
[5]. L.A. Bulavin, A.V. Chalyi, Springer Proceedings in Physics, **197**, 253, 2018.

11-9.O

SURFACE ABSORPTION OF LIQUID AT THE AIR-LIQUID INTERFACE

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Abstract: Surface tension is one of the most important properties of liquid. A new theory is proposed to describe the relationship between the surface tension and temperature for pure liquid compounds at constant pressure, and also the relationship between surface tension and concentrations of a solution at constant temperature and pressure. We found that relationship between the surface tension and temperature for pure liquid compounds is related to its phase transition from the bulk phase to the surface phase. The phase transition is exothermic and transition heats of 38 liquid compounds are determined quantitatively. This theory also describes successfully the variations of the surface tensions with the concentrations of solutes in strong electrolyte solutions at constant temperature and pressure. As a byproduct, minimum thicknesses of the surface layers of these solutions are deduced.

Reference

[1]. Feiwu Chen, Qing Ren, Novel surface absorption behavior of liquid at the air-liquid interface, *Chem. Phys. Lett.* **2017**, 685, 438–441.

[2]. Feiwu Chen, Tian Lu, Zhao Wu, Surface absorption of a solution at equilibrium, *Acta Phys.-Chim. Sin*. **2015**, 31, 1499-1503.

11-10.O

ISOTROPIC-NEMATIC TRANSITION AND DEMIXING BEHAVIOUR IN BINARY MIXTURES OF HARD SPHERES AND HARD SPHEROCYLINDERS CONFINED IN DISORDERED POROUS MEDIUM

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We generalize the scaled particle theory for the description of thermodynamic properties of a binary mixture of hard-sphere colloids and spherocylinder-like nematogenic nanoparticles confined in a disordered porous medium. The analytical expressions for the free energy, the pressure and the chemical potentials of hard spheres and hard spherocylinders are derived. We improve the obtained results by introducing the Carnahan-Starling-like and Parsons-Lee-like corrections. From the minimization of free energy the nonlinear integral equation for the orientation singlet distribution function is obtained. The phase diagrams of isotropic-nematic transition are calculated from the bifurcation analysis of this equation and from the condition of thermodynamic equilibrium. Both the approaches correctly reproduce the general trends of isotropic-nematic transition at small concentrations of hard spheres. However, the thermodynamic approach predicts the demixing transition at higher concentrations of hard spheres, but it is not available in the bifurcation analysis. The effects of disordered porous matrix on the isotropic-nematic and demixing transitions are discussed in terms of the total packing fraction of a mixture and the concentration of hard spheres for each of the coexisting phases. We show that a decrease of the matrix porosity shifts the region of isotropic-nematic coexistence towards lower packing fractions of a mixture. Simultaneously, this region gets narrower. For the case of long spherocylinders we observe that the system enters the demixing regime at lower hard sphere concentrations in matrices with the small porosity. The existence of upper limit packing fraction of a mixture is found at some matrix porosities. The obtained phase diagrams are in a good agreement with existing computer simulations data.

References

[1] M. Hvozd, T. Patsahan, M. Holovko, *J. Phys. Chem B*, (2018). DOI: 10.1021/acs.jpcb.7b11834.
[2] M. Holovko, T. Patsahan, M. Hvozd, *J. Mol. Liquids* (in press).

11-11.O

INTERPARTICLE INTERACTIONS AND DYNAMICS IN SOLUTIONS OF COPPER (II), COBALT (II) AND ZINC (II) TETRAFLUOROBORATES IN ACETONITRILE AT 5-55 °C

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This work is a continuation of the systematic study of unsymmetrical electrolytes in non-aqueous media, carried out at the Department of Inorganic Chemistry of V.N. Karazin Kharkiv National University [1].

Here we report the results of the conductometric study of diluted solutions of $Cu(BF_4)_2$, $Zn(BF_4)_2$ and $Co(BF_4)_2$ in acetonitrile (AN) at 5-55 ^oC. The extended Lee-Wheaton equation was used to procced conductometric data and obtain primary association constant of $M(BF_4)^+$, limiting equivalent conductance of electrolyte $\Lambda_0\left[\frac{1}{2}(M(BF_4)_2)\right]$ and limiting conductivities of $\frac{1}{2}(M^{2+})$, BF_4^- and $M(BF_4)^+$. The primary association constants were then used to interpret the contribution of the ionic solvation and association in terms of contact ionic pairs, solvent-separated ionic pairs and short-range non-Coulomb interionic potential.

Obtained values of total limiting equivalent conductivity of electrolyte $\Lambda_0\left[\frac{1}{2}(M(BF_4)_2)\right]$ and the limiting conventional transference numbers $t^0(M^{2+})$ allowed us to divide the equivalent conductivity on ionic constituents. These data were later proceeded to evaluate the parameter of dynamics of ionic solvation, within the modified theory of the dielectric friction.

Additionally, densimetric study was carried out to derive structural parameters of ion solvation of $Cu(BF_4)_2$, $Zn(BF_4)_2$ and $Co(BF_4)_2$ in AN at 5-65 ^oC.

Finally, molecular dynamics simulations were performed on the same electrolyte/AN systems by means of MDNAES package [2] to elucidate particle dynamics and microscopic structure within the first and second co-ordination shells of copper (II), cobalt (II) and zinc (II) cations in AN at 25 °C.

References

[1] O.N. Kalugin, V.N. Agieienko and N.A. Otroshko, *J. Molec. Liquids*, **165**, 78-86 (2012).

[2] O. N. Kalugin, M. N. Volobuev, and Y. V. Kolesnik, *Khar. Univ. Bull., Chem. Ser.* **454**, 58-80 (1999).

Poster session

11-1.P

A VESICLE-TO-SPONGE TRANSITION *VIA* PROLIFERATION OF PUNCTURES

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A nonlamellar lipid phase containing an omega-3 polyunsaturated fatty acid is dispersed into nanoscale objects in excess aqueous medium with the help of a PEGylated lipid. We investigated the self-assembled 3D nanostructure generation in diluted dispersions of the nonlamellar lipid mixture by small angle X-ray scattering (SAXS) and cryogenic transmission electron microscopy (cryo-TEM) microscopy. The included PEG-polymer lipid influenced the curvature of the mixed lipid assemblies loaded with an omega-3 fatty acid. High resolution SAXS permitted to study the proliferation and sizes of the aqueous channels in the PEGylated nanocarriers and the internal nanostructure transition. Cryo-TEM imaging revealed the morphological changes upon the transformation of the vesicular membranes into spongosome nanoparticles.

SMALL-ANGLE NEUTRON SCATTERING INVESTIGATION OF CO-DOPED IRON OXIDE NANOPARTICLE SUSPENSIONS

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Nanoferrites doped with cobalt are of special interest because of their large anisotropy and moderate magnetization, chemical stability and high value of Currie temperature [1].
Preliminary structural investigations on stable aqueous suspensions of several cobalt doped ferrites (CoxFe3-xO4, x=0; 0.5; 1) nanoparticles prepared by chemical co-precipitation method [2], are reported in the present work.
Small angle neutron scattering (SANS) measurements (Figure 1) [5] were performed at the time-of-flight YuMO spectrometer [3, 4] in function at the high flux pulse IBR-2 reactor, JINR Dubna.
Structural parameters of the samples are determined and discussed.

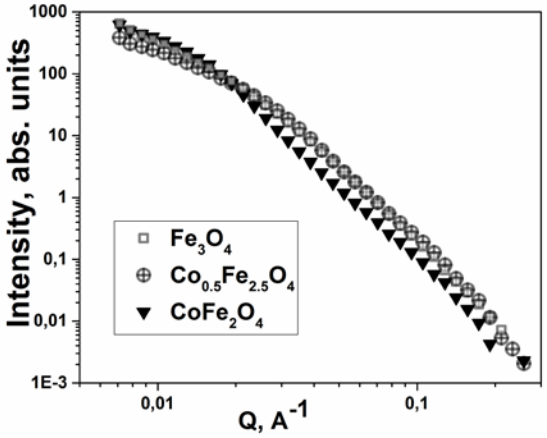

Figure 1. SANS experimental curves c cobalt doped ferrites (CoxFe3-xO4, x=(0.5; 1) samples.

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References

[1] M. Colombo, S. Carregal-Romero, M. F. Casula, L. Gutiérrez, M. P. Morales, I. B. Böhm, J. T. Heverhagen, D. Prosperi and W.J. Parak, Chem. Soc. Rev., 41, 4306 (2012)
[2] G. Tiriba, M. Balasoiu, E. Puscasu , L. Sacarescu, C. Stan, D. E. Creanga, U.P.B. Sci. Bull. Series A, 79(4) 327 (2017).
[3] A.I. Kuklin, A.K. Islamov, V.I. Gordeliy, Neutron News, 16(3) 16 (2005).
[4] A I Kuklin, A I Ivankov, D V Soloviov, A V Rogachev, Yu S Kovalev, A G Soloviev, A Kh Islamov, M Balasoiu, A V Vlasov, S A Kutuzov, A P Sirotin, A S Kirilov, V V Skoi, M I Rulev and V I Gordeliy, Journal of Physics: Conference Series, (2018) (to be published).
[5] D. Creanga, M. Balasoiu, D. Soloviov, A.-M. Balasoiu-Gaina, E. Puscasu, N. Lupu, C. Stan, Journal of Physics: Conference Series, (2018) (to be published).

11-3.P

SMALL ANGLE X-RAY STUDY OF CELLULOSE NANOCRYSTALS AND NANOFIBERS

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Morphological and dimensional characteristics of cellulose nanocrystals (CNC) and cellulose nanofibers (CNF) was investigated by small angle X-ray scattering (SAXS). To determine a shape and geometrical parameters of CNC and CNF several approximation models were applied to a measured data. Namely, these models are Guinier approximation [1], model of long rods with rectangular cross section [2], unified function model[3], Gaussian-approximated parallelepiped model[4].
Comparison of models shows that smallest deviation on original data gives model described in [2] and [4]. Both of models describe scattering on rectangular particles.
Height and width of CNC and CNF were determined, however, using given models it's impossible to determine a length of nanoparticles if other methods (such as SANS) are not applied [4].
Determined values in average for CNC are 3x16 nm and for CNF 2x12 nm. This result is in agreement with AFM data for same samples.

References

[1] M. Khandelwal and A. H. Windle, Int. J. of Bio. Macromolecules, 68, 215-217 (2014).
[2] O. M. Astley et al., Int. J. of Bio. Macromolecules, 29, 193-202 (2001)
[3] G. Beaucage, Combined small-angle scattering for characterization of hierarchically structured polymer systems over nano-to-micron meter: part II theory (2012)
[4] Y. Mao et al., J.Phys.Chem.B, 121, 1340-1351 (2017)

11-4.P

SPATIAL DISTRIBUTION OF THE ELECTRONIC EXCITATIONS GENERATION IN WATER WITH NANOPARTICLES OF GOLD UNDER X-RAYS IRRADIATION

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One of the major problems of the photodynamic therapy in medicine is lack of selective absorbtion of x-rays in organism exactly where it is requiered. The chemical compositions of different biological tissues (except bones) are almost the same, so the absorbtion coefficients are also similar within whole energy range. The problem could be solved by selective input of nanoparticles of gold into the organism as they have comparatively large absorbtion coefficient.
The main task of this project was to find the spacial distribution of the electronic excitations generation in water with nanoparticles. To do this, different processes of x-rays and matter interaction were studied, photoabsorbtion of gamma quantum in water and in gold, and generation of electronic excitations after absorbtion.

INCORPORATION OF WATER INTO CITRATE SHELL OF Au NANOPARTICLES SHELL: NEUTRON REFLECTOMETRY STUDY

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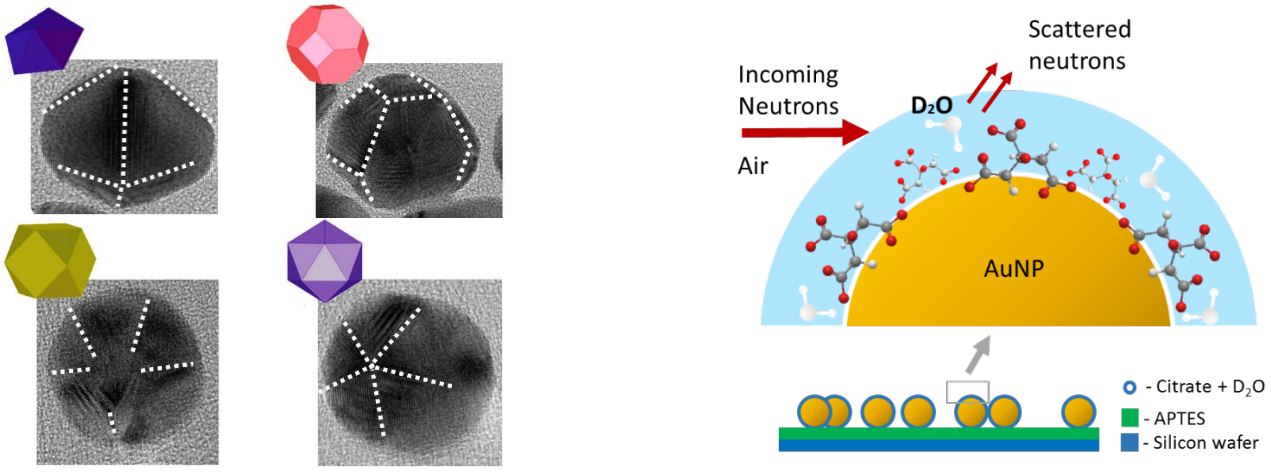
Optically active gold nanoparticles were synthesized in accordance with the modified Turkevich protocol using light water, H_2O, (AuNp-H) and heavy water, D_2O, (AuNp-D). A partial replacement of H_2O with D_2O resulted in some increase in the mean particle diameter (18.6 nm against 17.5 nm). The majority of AuNp in the two types of suspensions shows close to spherical form as evidenced by transmission electron microscopy (TEM). At the same time, high-resolution transmission electron microscopy (HRTEM) revealed different morphology of nanocrystallites of AuNp-H and AuNp-D (Fig.1a). This difference is considered to be one of the factors that is responsible for different optical properties of the solutions. Another factor is the difference in the dielectric constants of surrounding media of AuNp-H and AuNp-D, which is higher for the latter type of particles.



a) b)

Figure 1. HRTEM images of several selected AuNp-D with different nanocrystals structures, b) Schematic model of AuNp-D precipitated on silicon wafer with following drying.

From the analysis of the isotope effect for AuNp-D anchored on a silicon surface via APTES molecules, it was found that water and presumably citrate molecules form an organic shell around positively charged metallic core during the synthesis. As evidenced by neutron reflectometry (NR), water molecules remain in the shell after nanoparticle have been dried on the solid surface (Fig.1b). We suppose that when higher content of heavy water is used in the synthesis of the nanoparticles a stronger impact of crystallinity of AuNp-D on the optical properties of the suspensions is expected as compared to AuNp-H. Moreover, larger content of heavy water in the synthesis might give more molecules incorporated into citrate shell coating AuNp which widens the possibilities for the structural monitoring by NR. We also believe that the Turkevich protocol with light/heavy water substitution holds much promise for the NR characterization of complex materials based on liquid crystal, biological media or other multicomponent systems mixed with AuNp.

11-6.P

QUANTUM-MECHANICAL MODEL OF PHASE-CONTRAST IMAGES FOR LIQUID SYSTEMS

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X-ray imaging is one of the most powerful tools for investigating properties of non-crystalline objects, in particular, liquids and liquid systems. Among the different ways of obtaining x-ray images, the phase contrast imaging based on the triple-axes scheme with an analyzer (ABI — analyser-based imaging) is worthy of note because of relative simplicity and ease of realization. Although many methods to restore the characteristics of the object using its phase-contrast images have been proposed for today, all of them have some difficulties in obtaining stable solutions.
In this work, the approach based on the development of the quantum-mechanical theory of multiple scattering in both the object and the single-crystals of the monochromator and the analyzer have been proposed. The generalized theoretical model of phase contrast formation of inhomogeneous non-crystalline objects with arbitrary shape by triple-axes method have been developed by authors. The dispersion mechanism of the mutually consistent effect of the structure under study not only on absorption, but also on refraction, diffraction and extinction of radiation, due to multiple scattering, was taken into account analytically for the first time. The model takes into account self-consistently and analytically the effects of total X-ray multiple scattering at both on the homogeneous on average components of potential of the objects, and, for the first time, on the fluctuation one. The complete multiplicity have been taken into account in both the single-crystal of the monochromator and the analyzer, and in the object under study. The interrelation between the properties of the object under study and the experimentally observed parameters of the distribution of the rays intensities was analytically established.

WORKSHOP: Radiative Aspects of the Physics of Liquid State.

Oral session

10-1.O

THE RADIO-ADAPTIVE RESPONSES IN LIQUID BIOLOGICAL SYSTEM OF *CAENORHABDITIS ELEGANS* MEDIATED BY INTRA- AND INTER BYSTANDER SIGNALS

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Though radio-adaptive response (RAR) and radiation induced bystander effects (RIBE) are two important aspects for evaluation of low-dose radiation hazardous in the environmental condition, there are currently only limited data that directly address their interaction, particularly in the context of whole organisms. In the current study, we investigated the interaction of RAR and RIBE in *C. elegans* with the ratio of protruding vulva as the biological end point. By doing this, fourteen-hour-old worms were first locally targeted with a proton microbeam, and were then challenged with a high dose of whole-body gamma radiation. Our results showed that microbeam irradiation of the posterior pharynx bulbs and rectal valves of *C. elegans* could significantly suppress the induction of protruding vulva by subsequent gamma irradiation, suggesting a contribution of RIBE to RAR in the context of the whole organism. Furthermore, we investigated the RAR mediated by RIBE between worms through volatile signals in the liquid environment by establishing a co-culture experimental system using *C. elegans* in a top-bottom layout, where communication between top and bottom worms was airborne. It was shown that γ irradiation of bottom worms initiated RAR in top worms, and deficiency in ascaroside biosynthesis prevented the production of the volatile signals in a population-dependent manner, suggesting an inherent link between waterborne and airborne communications. The above results indicated an important role of liquid environment in the RIBE-mediated RAR in intra- and inter-worms.

10-2.O

NUCLEAR SPIN CATALYSIS AND STABLE MAGNETIC ISOTOPES AS NEW TOOLS FOR ANTI-RADIATION MEDICINE

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Once atomic power engineering has become a part of our everyday lives, the special precautions should be taken to defend the people in case of chronic radiation. Novel anti-radiation protectors are required which would be non-toxic and suited to long-time applications. Of special interest, can be stable magnetic isotopes of some chemical elements which normally present in nature. Among three stable isotopes of magnesium, ^{24}Mg, ^{25}Mg, and ^{26}Mg, with natural abundance 76.7, 10.1 and 11.2 percent, ^{25}Mg is magnetic (nuclear spin I = 5/2) while ^{24}Mg and ^{26}Mg are nonmagnetic (I = 0). The beneficial effects of ^{25}Mg have been discovered in the post-radiation recovery of yeast cells, *S. cerevisiae*, after X-ray irradiation. The cells enriched with magnetic ^{25}Mg demonstrate two-fold increase in the rate constant of post-radiation recovery as compared with the cells enriched with nonmagnetic ^{24}Mg. At this, the fraction of the irreversible damages in the cells enriched with ^{25}Mg is 60 percent less than in the cells enriched with ^{24}Mg [1]. In experiments with myosin, the important molecular motor of cell bioenergetics, it was revealed that the enzymatic ATP hydrolysis proceeds 2.0-2.5 times faster with magnetic ^{25}Mg than with the nonmagnetic isotopes [2]. Similarly, the rate of the ATP hydrolysis driven by myosin with magnetic zinc isotope, ^{67}Zn (I = 5/2), is 40-50 percent higher as compared to nonmagnetic ^{64}Zn or ^{68}Zn. Plausible biophysical mechanisms of the nuclear spin catalysis are discussed in [3]. Thus, there are the grounds to believe that ^{25}Mg and some other stable magnetic isotopes hold much promise in creating novel anti-radiation protectors.

References

[1] V.K. Koltover, T.A. Evstyukhina, V.G. Korolev and Y.A. Kutlakhmedov, *Europ. Biophysics J.*, **46**, 317 (2017).
[2] V.K. Koltover, R.D. Labyntseva, V.K. Karandashev and S.O. Kosterin, *Biophysics*, **61**, 200-206 (2016).
[3] V.K. Koltover, *J. Mol. Liquids*, **235**, 44-48 (2017).

10-3.O

BIOEQUIVALENT DETECTORS OF IONIZING RADIATION AND BIOLOGICALLY ACTIVE UV

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Efficient and reliable detectors of ionizing radiation is a long-standing problem that re-emerges from time to time after accidents at nuclear power plants and other contingencies. The existing scintillation and semiconductor detectors are generally adequate in most cases, though some problems remain, e.g., in detection of weak and low-energy radiation. Also, since the response mechanism of solid-state detectors is essentially different from radiation-induced processes in living tissues, it is sometimes not easy to correlate the measured exposure or absorbed dose with expected biological effects. In our studies, we used liquid crystals (LC) as a model medium to mimic the radiation effects. In fact, effects of radiation on lyotropic liquid crystal state of cell membranes can be easily studied with conventional physico-chemical instrumental means, reflecting changes in molecular structure, and the mechanisms involved can be reproduced in artificial LC structures ensuring both bioequivalence and high sensitivity. A review of the obtained results is presented, and advantages of the proposed approach are most clear for low-energy radiation of weak intensity. The same approach was later generalized for detection of biologically active UV radiation, which appear to be most suitable for assessment of the accumulated dose in the range close to the UVB/UVC boundary. Physico-chemical evidence is presented, showing the similarity of radiation-induced changes on molecular and supramolecular level in model liquid crystal structures and certain biological tissues.

10-4.O

RADIATION INFLUENCE ON THE TEMPERATURE-DEPENDENT PARAMETERS OF FLUIDS: THEORY AND COMPUTER SIMULATION

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The work is devoted to the self-consistent study of the radiation influence on the structure and thermophysical properties of fluids that includes both theoretical study and molecular dynamics simulation.
Within the suggested approach it is assumed that the structural changes in the liquid systems under irradiation are caused by the changes in the coefficients of the Maxwell distribution function due to the momentum exchange between the active particles and the particles forming the liquid. To quantify this the theoretical model based on the fundamental Bogolyubov chain of equations and relating the structural and thermophysical properties of the nonequilibrium liquid systems under irradiation in stationary state is introduced [1]. The obtained results suggest that the thermophysical properties of the liquid systems under irradiation are defined by the new parameter "effective temperature" that can be calculated from the perturbed momentum distribution functions of the systems. The qualitative comparison of the model predictions with the existing experimental data on irradiation influence on the surface tension coefficient of liquids suggests that the obtained results are in accord with the experimental data.
The conducted computer simulation of the irradiation influence on water shows the changes in the radial distribution functions, momentum distribution function and the selfdiffusion coefficients under the irradiation. It is shown that the irradiation causes the changes in the structural and thermodynamic properties of water. The developed theoretical model is used to explain the phenomena observed in the molecular dynamics simulation. It is shown that the suggested theory is able to quantitatively explain the observed changes in the water properties.

References

[1] L. A. Bulavin, K. V. Cherevko, D. A. Gavryushenko, V. M. Sysoev, and T. S. Vlasenko, *Phys. Rev. E,* **93**, 032133 (2016).

10-5.O

NUCLEAR AND RADIATION ACCIDENT EMERGENCY PREPAREDNESS AND RESPONSE IN CHINA

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Emergency Preparedness and Response (EPR) has become a hot topic for its significant role in nuclear safety. In this talk, Firstly, I will introduce the regulatory framework, including regulatory body and its TSOs, legal system in China. Then, management system for nuclear and radiation accident emergency preparedness and response as well as environmental radiological monitoring in China will be presented. In addition, the national EPR center, Nuclear and Radiation Accident Emergency Technical Center (ETC) for Ministry of Ecology and Environment will be introduced. Finally, I will describe some classical response and exercises supported by ETC with different scenarios.

10-6.O

ON THE EFFECT OF EXTERNAL STOCHASTIC FIELD ON SYSTEMS OF PARTICLES INTERACTING WITH MULTIPLYING AND CAPTURING HYDRODYNAMIC MEDIA

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This work considers dynamics of non-equilibrium long wave fluctuations in systems of particles interacting with multiplying and capturing media, generated by external stochastic field. General dynamic equations for long wave fluctuations are obtained using the method of averaging over external random force. The case of additive Gaussian noise is considered in detail. It is shown that in the case of such an external random force there exists a time interval during which the description of the evolution of the system can be limited to considering only the dynamics of the hydrodynamic pair correlations. Linearised dynamic equations for pair correlations are obtained, and their solutions in case of small spatial inhomogeneity are considered. The formation of stationary states and the problem of their stability is studied. It has been shown that long wave fluctuations can be generated by external random force and dramatically influence on stability of stationary states in some cases.

10-7.O

STUDY ON THE FUNCTION OF YTIB & YTHA GENE OF BACILLUS ATROPHAEUS ON URANIUM REMOVAL

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Two Bacillus atrophaeus strains, ATCC 9372 strain which is a standard strain with a high resistance to stress, and Ua strain which was screened out from a chromium mine in my lab, have different tolerabilities and removal capacities to U(VI). With the U(VI) concentration increasing, the tolerability and bioremedial capacity of both the strains to U(VI) decrease. But the ATCC 9372 strain has a better U(VI) tolerability and removal capacity than the Ua strain. In order to study their gene difference, the pulsed-field gel electrophoresis (PFGE) method was used, and transgenic technology was performed to verify the relationship between different genes and U(VI) removal capacity. One different DNA band of 3128 bp in Ua strain, digested with EcoRI and HindIII endonuclease together, separated by PFGE, was selected for studying. While analyzing the different DNA band sequences it is found that there are a ythA gene and a ytiB gene, and the sequence of both the left and right ends corresponds with the restriction enzyme cutting site of EcoRI endonuclease and HindIII endonuclease, respectively. PCR verification test also indicates that the ytiB gene exists only in the Ua strain. Using pBE-S DNA(TAKARA) as vector, the ytiB gene and ythA gene were transferred into Bacillus atrophaeus ATCC 9372 strain respectively. Under the U(VI) concentration of 120 mg/L, the removal rate of the ATCC 9372-ytiB (ATCC 9372 strain transferred with ytiB gene) strain and ATCC 9372-ythA (ATCC 9372 strain transferred with ythA gene) strain are decreased by 7.55% and 7.43%, respectively, which indicate that the ytiB gene and ythA gene have a negative effect on U(VI) removal function. Therefore, ythA gene and ytiB gene have an evident lower influence on uranium removing, and the pulsed-field gel electrophoresis (PFGE) is a good method to study gene difference.

10-1.P

Zr AND Hf PHTHALOCYANINE COMPLEXES WITH KETOENOLE LIGANDS: SOLVENT DEPENDENCE OF INTRAMOLECULAR ENERGY TRANSFER EFFICIENCY

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Compounds able to absorb UV and visible light in the widest possible range could be applied in a variety of devices (e.g. solar cells). Here we report the spectral-luminescent study of Zr and Hf phthalocyanine complexes containing β-ketoenole ligand (Fig. 1). Absorption spectra of both compounds (Fig. 2) in polar acetonitrile as well as in non-polar toluene consist of the bands corresponding to transitions in phthalocyanine (Soret band - 345 nm and Q-bands - 620 nm and 685 nm) and in β-ketoenole ligand (near 445 nm); these spectra are similar for both compounds in both solvents. For non-polar toluene solutions, it is seen from the fluorescence excitation spectrum (Fig.2) that the phthalocyanine fluorescence (emission at 710 nm) is induced by excitation into all the mentioned absorption bands, including the one of β-ketoenole ligand. This means that excitation energy transfer from β-ketoenole ligand to phthalocyanine core takes place (with estimated efficiency of about 70% for Zr-containing compound).

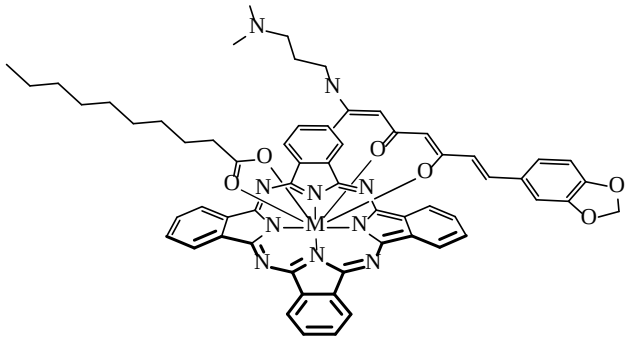

Fig. 1. Structure of the studied compounds. M stands for either Zr or Hf ion.

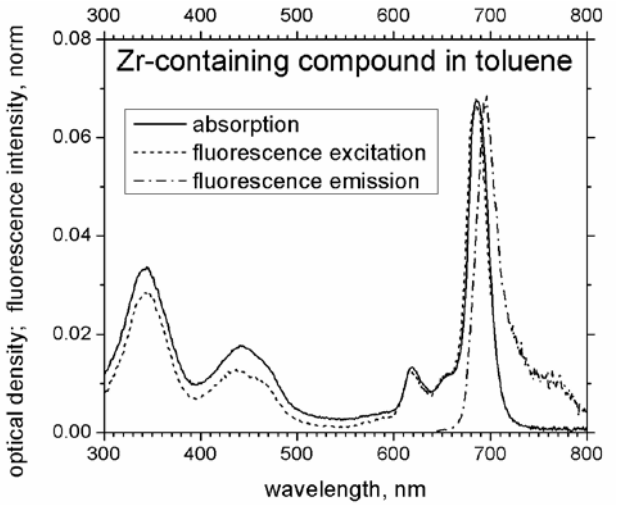

Fig. 2. Absorption, fluorescence excitation (emission at 710 nm) and emission (excitation at 360 nm) spectra of toluene solution of Zr-containing compound.

Meanwhile, in polar acetonitrile solution there is no evidence of any energy transfer from β-ketoenole ligand to phthalocyanine core. We believe this could be connected with the fast non-radiative excited state relaxation of β-ketoenole molecule in polar acetonitrile medium.

Thus the studied complexes in non-polar medium are able to absorb light at wide spectral range from 300 to 700 nm (though with low absorption between 500 and 600 nm) and transfer this energy to the phthalocyanine core which could be further used.

Acknowledgements

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10-2.P

ELLIPSOMETRICAL DIAGNOSTIC OF METAL-DIELECTRIC STRUCTURES WITH SURFACE GRAPHENE LAYER

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The features of optical properties of graphene films grown at two temperature modes on different Cr- Cu - HfO_2 heterostructures using chemical vapor deposition method were investigated via spectral ellipsometry measurements. These measurements were performed applying Beattie technique. The azimuth ψ of the restored linear polarization and the phase shift Δ between *p*- and *s*- components of polarization vector were measured at different values of light incidence angle φ on the sample from 45^o to 85^o by step of 5^0 and at different azimuthal angles α changing in own sample plane at the fixed φ value from 0^o to 360^o by step of 5^0 . Ellipsometric parameters ψ and Δ are defined from ellipsometry equation $\tan \Psi \exp(i\Delta) = r_p / r_s$. Measurements have been performed consistently for the substrate and relatively large size samples, and then the results were modeled by method based on the Fresnel coefficients for semi-infinite medium. Azimuthal angle α variable ellipsometry measurements were performed to analyze the polar dependence of both ellipsometric parameters ψ and Δ to estimate the appropriate optical anisotropy in own plane of heterostructures. The significant enhancement of the absorption band in the graphene layers positioned with respect to the bulk graphite spectral range due to response of the exited surface-localized plasmons in thin film as Cr-Cu-HfO_2 – Graphene were observed. The obtained results provide direct evidence of the strong influence of a specificity of morphology of surface on electronic structures and optical properties of the sample with graphene layer.

10-3.P

DEPENDENCE OF THE CONCENTRATIONS OF CESIUM-137 AND POTASSIUM IN EXTRACTED SOIL SOLUTIONS ON SOIL HUMIDITY BEFORE CENTRIFUGATION

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The most important factor for Cs-137 transfer from soil to plant is content of Cs-137 and potassium in the soil solution. The concentrations of cesium-137 and potassium in solutions extracted by centrifugation from soils selected at experimental sites in the 10-km Exclusion Zone of Chornobyl Nuclear Plant were determined. Experiments were performed during 2012 and 2013 years at four field sites with different types of soil. Samples of the soils were selected several times during the every growth season. Values of soil humidity were determined for each of the selected soil sample. The experimental conditions were described in details elsewhere [1]. The obtained data showed that, for the majority of the soils investigated, the concentration of cesium-137 in the soil solution depends on the humidity of the soil before centrifugation. It is possible to explain this dependence from the dependence of the concentrations of molecules of different molecular-gravimetric fractions in the soil solution on soil humidity. A considerable amount of cesium-137 in the soil solution is associated with these molecules, which is why the concentration of cesium-137 in the extracted soil solution changes with the humidity of soil. These dependences differ between soils. For the majority of soils investigated the concentration of cesium-137 in the extracted soil solution increases with increasing humidity of the soil. By contrast, soil humidity had no effect on the potassium concentration in the extracted soil solution for any soil investigated. It is concluded, therefore, that little potassium is associated with the mentioned molecules of molecular-gravimetric fractions in the extracted soil solutions.

References

[1] V. Prorok, O. Dacenko, L. Bulavin, L. Poperenko, and P. White. Journal of Environmental Radioactivity, 152 (2016) 85-91

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NANOSTRUCTURED SOLID/FLUID INTERFACE CHARACTERIZATION WITH PHOTOACOUSTIC TECHNIQUE

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Nanostructured materials with an important specific surface are promising for their application in different fields of nano-, optoelectronics, biology and medicine [1,2]. The use of nanomaterials as constituent components of various composite systems with solid / fluid interfaces is significant for various applications. Therefore, understanding of interfacial phenomena at the nanostructured solid/fluid interface in the cases of the lyophilic and lyophobic surfaces is crucial for performance stability and reliability of nano/micro devices [3]. It should be noted that the presence of nanoscaled features with large curvatures is defining factor for modification of physic-chemical properties at the interface.

Our report is devoted to the photoacoustic characterization of nanostructured solid/fluid interface. In our study lyophilic and lyophobic surfaces were considered. The photoacoustic signal was recorded in a piezoelectric configuration. Amplitude-frequency dependencies of the photoacoustic responses from multilayered structure were experimentally measured. The photoacoustic response shapes in the cases of presence and absence of a surface liquid covering layer in contact with the nanostructured surface was experimentally detected. Modification of the response shape caused by existence of "nanostructured solid / liquid" interface was analyzed.

References

[1] B. Van Grinsven, N. Vanden Bon, H. Strauven, L. Grieten, M. Murib, S.D. Janssens, K. Haenen, M.J. Scho, K.L. Jime, V. Vermeeren, M. Ameloot, L. Michiels, R. Thoelen, W. De Ceuninck, P. Wagner, Heat-Transfer Resistance at Solid- Liquid Interfaces : A Tool for the Detection of Single-nucleotide Polymorphisms in DNA, ACS Nano. (2012) 2712–2721.

[2] M.S. Muthu, D.T. Leong, L. Mei, S.S. Feng, Nanotheranostics - application and further development of nanomedicine strategies for advanced theranostics, Theranostics. 4 (2014) 660–677. doi:10.7150/thno.8698.

[3] Z. Ge, D.G. Cahill, P. V Braun, Thermal Conductance of Hydrophilic and Hydrophobic Interfaces, Phys Rev Lett. 96 (2006) 186101. doi:10.1103/PhysRevLett.96.186101.

ON MATHEMATICAL ALGORITHMS FOR THE RELIABLE RADIOACTIVE COMPONENTS IDENTIFICATION FROM THE SPECTROMETRY DATA

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The presented results deal with the development of the reliable algorithms for the radionuclide identification from the gamma spectra. The analysis of the matching pursuit (MP) method that is the representative of the family of sparse approximation approaches to signal processing has been studied and modified in order to be able to decrease the dimensionality of the model without losing the real signals. It is analyzed the possibility to use the stopping conditions incorporating the Gribonval l0-optimality criteria for the matching pursuit algorithms. The new conditions may allow using the DRF as the basis functions.
The possible advantages of the implementing the blind source separation (BSS) method incorporating the fundamental relations of the algorithmic information theory for the radionuclide identification are studied. The new approach to the unknown source identification based on the classical blind source separation (BSS) method was proposed. Fundamental relations of the algorithmic information theory were used to develop the novel BSS method with the target function being the minimal description length (MDL) in different forms. The possibility to use the detector response functions as the basis functions in the iterative procedure of the BSS method with the target function being the minimal description length was studied.
Algorithms and basic software modules of the MP approach with the Gribonval l0-optimality stopping condition and BSS-MDL method have been developed. The developed modifications of the MP and BSS methods have been tested on the artificial signals.
The suggested algorithms might be used for detecting the radionuclide in the contaminated liquids.

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