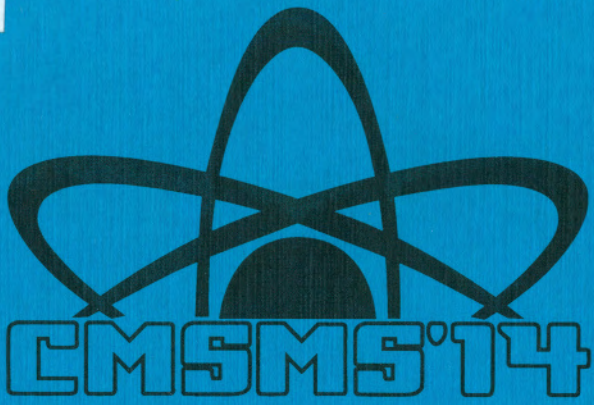

2nd International Summer School and Workshop

COMPLEX AND MAGNETIC SOFT MATTER SYSTEMS: PHYSICO-MECHANICAL PROPERTIES AND STRUCTURE

29 September – 3 October 2014, Dubna

Book of Abstracts

JOINT INSTITUTE FOR NUCLEAR RESEARCH

CMSMS'14

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Preface

On behalf of the International Advisory Committee, Program and Local Organizing Committees we welcome you to the 2nd International School and Workshop on Complex and Magnetic Soft Matter Systems: Structure and Physico-Mechanical Properties (CMSMS'14).

The CMSMS 2014 is organized by Joint Institute for Nuclear Research (Dubna), West University of Timisoara, Institute of Continuous Media Mechanics of Russian Academy of Sciences (Perm), Institute of Physics and Nuclear Engineering "Horia Hulubei" (Bucharest) and Romanian Society of Physics.

The Organizing Committee is very grateful to Romanian Plenipotentiary to JINR, to Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research, Russia, to West University of Timisoara, Romania, to the firm Frako-Term Sp. z o.o., Poland for the financial support of the CMSMS'14.

The topics of lectures, oral and poster presentations cover the theory, simulations, and experimental research in physical, mechanical, structural and chemical aspects of the materials science as well as biological aspects of soft complex matter with special emphasis on soft magnetic matter (magnetic elastomers, ferrogels, ferroliquid crystals, associations of nanoparticles with biomolecules and cells, etc.).

The first International Summer School and Workshop "Complex and Magnetic Soft Matter Systems: Physico-Mechanical Properties and Structure" (CMSMS'12) took place from 3 to 7 September 2012 in Alushta (Crimea). It has brought together 32 specialists (top-level experts and young researchers) from Russia, Romania, Moldova, Belarus, Ukraine, France and Germany working on interdisciplinary problems in soft matter. Their contributions totaled 37 works.

The main objective of CMSMS'14 is to exchange the latest research findings in the scope of the meeting. More than 60 pre-registered authors submitted their contributions. CMSMS'14 would offer a number of invited lectures delivering a concise overview of several important research issues in complex and magnetic soft matter and related fields. Young scientists were encouraged to present their results in oral talks. The poster sessions will extend the frame of oral sessions providing opportunities to continue the scientific exchange in personal discussions.

With all this, we hope that CMSMS'14 will be a successful and stimulating scientific event.

Program and Local Organizing Committee

Invited Lectures

An introduction to fractional exclusion statistics: thermodynamics and transport

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Real systems are not composed of ideal particles, so in order to describe them in a single-particle picture one has to define quasiparticles with conveniently chosen characteristics. Although these quasiparticles are useful in many cases, they are still interacting, i.e. they influence each-other's properties.

Here we show how general interacting particle systems may be described as ideal gases. In order to do this, one needs a method to define quasiparticle states with the property that the sum of quasiparticle energies is equal to the total energy of the system. But the key to succeed lays not only in the definition of the quasiparticle energies, but also in the perspective we have about the quasiparticle states and in the rules of counting them. The ideal gas thus obtained obeys neither the Bose, nor the Fermi occupation rules of the single-particle states but a generalization of these, called *fractional exclusion statistics* [1].

Further, we show how one can describe a mean field interacting particle system in any number of dimensions and in generic external potential as an ideal gas with fractional exclusion statistics [2] and how to describe the particle transport through such a system [3].

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Biogenic nanoparticles of ferrihydrites

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Previously it has been shown that ferrihydrite nanoparticles synthesized by Klebsiella oxytoca bacteria in the biomineralization of iron salt solutions from the culture medium [1,2] exhibit a unique magnetic properties: they are characterized by an antiferromagnetic order inherent in bulk ferrihydrite and spontaneous magnetic moment of the spins due to decompensation in nanoparticles sublattices. This paper presents the results showing that ferrihydrite nanoparticles are formed on the surface of the bacterial cell. The bacterial culture was grown in the Lovley medium, and then citrate buffer pH=5 (citric acid 40g / l, pH = 7 was set up by adding KOH) was added and further culture incubating during 1 to 25 hours was performed. The addition of citrate buffer in the culture medium did not significantly affects the number of viable bacterial cells in the medium, therefore, a citrate buffer does not destroys the cells. Upon the analysis of Mossbauer data we showed that after treatment of cell cultures with citrate buffer and washing the cells with the addition of NaCl there is no ferrihydrite nanoparticles in the suspension. This indicates that the nanoparticles were completely separated from bacterial cells. The above arguments lead to the conclusion that the ferrihydrite nanoparticles were synthesized on the cell surface of bacteria Klebsiella oxytoca.

Support by State Ministry of Education and Science is acknowledged.

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Neutron scattering instruments of IBR-2 reactor for condensed matter research. Current state and recent results

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Since the re-start of the regular operation of the IBR-2 high flux pulsed reactor after full-scale modernization in 2012, the complex of neutron scattering instruments installed at the reactor was substantially upgraded. It contains in total 14 instruments, including diffractometers, small angle scattering spectrometer, reflectometers, inelastic neutron scattering spectrometers. New instruments – DN-6 diffractometer for studies of microsamples under extreme conditions, GRAINS multifunctional reflectometer, neutron imaging facility were put into operation. A number of existing spectrometers was also modernized to improve technical parameters. An overview of the recently obtained scientific results and prospects for interdisciplinary research in the fields of condensed matter physics, materials science, chemistry, biophysical and geophysical sciences at IBR-2 neutron scattering instruments is presented.

Advances in neutron scattering from biomembranes

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Biological membrane mimetics, such as liposomes, lipid bilayers and model membranes, are used in a broad range of scientific and technological applications due to the unique physical properties of these amphiphilic aggregates. They serve as platforms for studying the soft matter physics of membranes and membrane dynamics, interactions of bilayers with drugs or DNA, and effects of various additives or environmental changes. The modern state-of-the-art research takes advantage of joining brilliance of X-ray scattering sources with some peculiar properties of neutrons, and combines results with the power of computer simulations. The advances in chemistry and deuteration possibilities in particular, allow for better experimental spatial resolution and possibility to pin-point labels within membranes. It is only a matter of time for various technological applications to follow these advances and utilize the amphiphiles in e.g., liposome-based nanoparticles for drug delivery, formulation of liposomes for prolonged *in vivo* circulation and functionalization for medical purposes, novel drug delivery systems for increased drug loading, and the use of tethered membranes for bio-sensing applications. The use of liposomes in textile dyeing, and a role of lipidic nanoparticles in the food industry is already happening future.

Ordering of mixed paramagnetic and diamagnetic fullerenols in aqueous solutions under magnetic field

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Aqueous solutions of the mixtures of paramagnetic $Gd@C_{82}(OH)_X$ and diamagnetic $C_{82}(OH)_X$ ($X \sim 30$) fullerenols (temperature 25°C) have been studied by polarized neutrons at various concentrations from diluted to concentrated systems close to the threshold of fullerenols solubility. As a result of increase of fullerenols content ($C = 0.04 - 2$ % wt.) and magnetic field application ($B = 0.001 - 1.0$ Tesla), there was detected a growth of molecular nano-sized correlations (radius R_C ~15-20 nm), when the aggregation number achieved the magnitudes ~ $5 \cdot 10^4$. These effects should be attributed to paramagnetic molecules as well as to the interactions of diamagnetic moments induced in fullerenols integrated. The polarized neutron experiments have shown that the concentrating of systems has not broken their stability at macroscopic level while nano-scale aggregates achieved high masses and at the next structural level showed the trends to association into superstructures (~ 500 nm in diameter). On the other hand, the fields $B \sim 1$ Tesla were not so strong to induce fullerenols' substantial magnetic ordering. This was confirmed by rather small contribution of nuclear-magnetic interference (≤ 0.1 %) to the total scattering cross section even at relatively high content of fullerenols ($C = 2$ % wt.). The established peculiarities of fullerenols' magnetic ordering in aqueous solutions with the variation of their concentration in a wide range seems to be important for the profitable opportunities of fullerenols' applications to solve biomedical tasks assuming the creation of new preparations for medical MRI-diagnostics and tumors' therapy [1,2].

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[2] Kozlov V.S., Suyasova M.V., Lebedev V.T. Synthesis, Extraction, and Chromatographic Purification of Higher Empty Fullerenes and Endoghedral Gadolinium Metallofullerenes. // Russian Journal of Applied Chemistry. **87**, 121 (2014).

Modeling of capacitor with magnetorheological media

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The effect of a uniform external magnetic field on the effective permittivity of magnetorheological elastomers (MREs) was simulated. It is considered that capacitance of plane capacitor filled with MRE and, thus, the effective permittivity of MRE is dependent on the external magnetic field. This effect is called magnetodielectric effect or magnetocapacitance effect in MRE. The model was developed to qualitative explain the experimental results obtained in [1].

The model was developed to analyze behavior of spherical equally sized magnetic particles uniformly distributed in elastic matrix under the external magnetic field. The change of capacitance of capacitor filled with MRE was calculated. We considered dipole-dipole interaction between particles. Particles were assumed as soft magnetic, so we put interaction of particles magnetic moments with external magnetic field only as orienting. We took Hooke's law, as particle-matrix interaction – each particle is connected with its initial position by ideal string.

The particles were shown to tend to the formation of chain-like structures when magnetic field is applied (Fig. 1), and the displacement of particles and, therefore, the value of magnetodielectric effect, was shown to be dependent on the elastic properties of matrix and intensity of magnetic field.

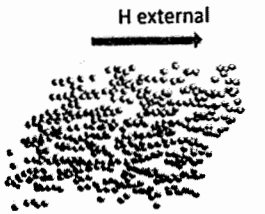

Fig. 1. Chain-like particles distribution in MRE formatted under applied external magnetic field.

Dependence on particles volume concentration was also simulated (Fig. 2).

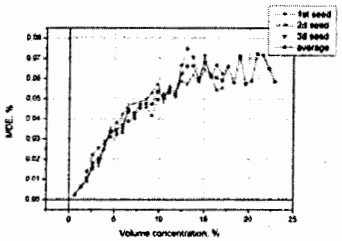

Fig. 2. Relative change of capacitance of capacitor filled with MRE vs. particles volume concentration for three different random particles distributions.

The observed field-induced phenomena evidence the attractiveness of MREs as novel promising materials in family of composite multiferroic materials.

Supported by RFBR (grants 13-03-00914, 13-02-90491, 13-02-12443).

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Modeling of particle interactions in magnetorheological elastomers

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The microparticle fillers of magneto-rheological suspensions (MRS) and MR-elastomers are multi-domain. This entails their quasi-linear magnetization in weak fields and saturation under strong ones. Being heavy enough, the particles are but slightly affected by Brownian motion, and weakly sensitive to colloidal interactions. Therefore, when an external field is imposed, the particle behavior is entirely defined by their magnetostatic interaction.

In dense systems, which are most interesting practically, the majority of the particles are separated by the distances counting just a small fraction of their diameter. Under such conditions, the interaction of the field-induced particle magnetic moments differs drastically from the usual dipole-dipole potential. The physical cause for that is the reciprocally induced non-uniformity of the *intra*-particle magnetization. This, in turn, affects the *inter*-particle forces, and, thus, the morphology and the magneto-mechanical response of a system.

In the theory, the problem of magnetostatic interaction of a pair of linearly polarizable particles has an exact (albeit quite cumbersome) solution [1]. Formally, the extension of this (linear) solution to the case of multi-particle assembly is also possible. However, in practice, it could hardly be advanced further that the three-particle-case [2]. These difficulties strongly compel one to use computer simulations. The more so, that any nonlinearity added to the problem—e.g. the ability of the particle magnetization to saturate—completely wipe out the possibility of analytical treatment. In the case of MRE there exist another essential source of strong nonlinearity. Any particle displacement in a polymer matrix in response to the ponderomotive forces, inevitably induces the restoring elastic forces. The latter, if to exclude the trivial case of Hookean elasticity, are always nonlinear.

To build up the modeling approach, we have first taken the case of two-particle subjected to a uniform external field. Instead of about one-hundred term series, which expresses the exact solution for the case of highly-polarizable (e.g. iron) particles, we propose a handy interpolation formula for the interparticle magnetic energy. Its coefficients are adjusted by comparison with the exact result and provide good accuracy within the range of interparticle separations, where the multipole expansion really matters. This interval is

not wide: in terms of the center-to-center distance it spans from $2a$ (tight contact) to $\sim 4a$, where a is the particle radius. On the other hand, the short-range interaction is important for understanding the nucleation of aggregates in the magnetic microparticle assemblies: from usual iron files visualizing magnetic fields to magnetorheological suspensions and magnetorheological elastomers (MREs).

At short distances, the forces by which magnetizable particles are coupled to one another differ significantly from the predictions of the point-dipole model. This concerns both the magnitude of the center-to-center force and its angular dependence. In fact, when such particles are in close vicinity of each other, the entirely dominating type of their coupling is attraction. This means that the emerging two-particle cluster might form not only from the particles, whose center-to-center vector is along the field, but also from those pairs which are tilted in a wide range of angles.

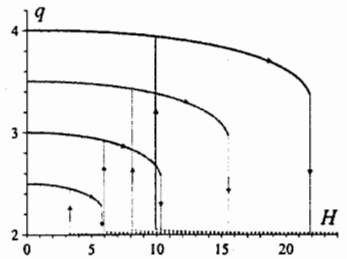
In a MRE is in the field-free and mechanically unloaded state, each microparticle rests in its equilibrium location and experience zero net force. When a magnetic field is imposed, the field-induced forces strive to organize (aggregate) the particles in the patterns which minimize the magnetic energy. The matrix reacts to this by generating the elastic counter-forces resisting the particle displacements. Therefore, the changes of internal particle structure as well as macroscopic deformations of a MRE sample occur as a result of balancing the magnetic and elastic energy increments.

To account for the situation, we considered the elastic energy contribution induced by mutual approach of two particles, whose center-to-center vector is parallel to the applied field. The matrix is assumed to be the Mooney-Rivlin medium that is a conventional way to describe mechanical properties of typical elastomers. This model is non-linear and thus does not admit exact solution. Solving the problem by finite-element method, we got the results in numerical form. To facilitate the main task—minimization of the summary magnetoelastic energy of the particle pair—we used the obtained numeric array as a basis for constructing an interpolation formula [3]. This expression seems to be robust for arbitrary interparticle separations except maybe for the direct surface contact of the particles.

Minimization of the summary energy reveals that in a certain field range the system becomes bistable. Of the two possible equilibrium states, one corresponds to weak compression of the pair, while the other energy minimum means close neighboring of the particles and, thus, strong deformation of the matrix. On further increase of the field, the "distant" (weak-deformation) minimum disappears, and the tightly collapsed (cluster) state

remains the only possible one. As soon as the cluster is formed, the interparticle distance becomes virtually independent of the field strength.

Under bistability conditions, the transitions between the equilibrium configurations of the pair occur in a hysteretic manner. Let the particle pair respond to turning on a weak field by a small deformation. Upon increase of the field, the system would reside in this particular state even after appearance of the second minimum because thermal fluctuations are negligible. The weakly deformed configuration would cease to exist only when the "distant" energy minimum disappears. As a result, the particles would necessarily move into the only remained "close" minimum thus forming a cluster. Under diminution of the field, the same scenario applies to the restoration of the initial state of the pair. In the figure a qualitative view of this magnetomechanical hysteresis is shown: the interparticle distance q is plotted against the applied field strength H. The area of the loops grows with the increase of the initial interparticle distance.



The bistability effect in a pair of magnetizable particles embedded in an elastic matrix is of apparent importance for MREs. It favors abundant clusterizing accompanied by shrinking of the sample in the direction of the field and a substantial change of rheology of the material.

The work is supported by RFBR grants #14-02-96003 and 13-01-96056, UB RAS Program #10 (12-P-01-108) and project MIG S26/617 from the Ministry of Education and Science of Perm Region.

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The magnetic spin diffusion barrier does it: Polarized proton spin clusters observed by time-resolved polarized neutron scattering from organic radicals of different size

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Motivated by potentially important applications in structural biology, experiments of time-resolved polarised neutron scattering from dynamic polarised proton spin targets were undertaken in order to elucidate the build-up of proton spin polarisation near paramagnetic centres. Organic radicals of different size like EHBA-CrV, DPPH and a biradical dissolved in a deuterated solvent were used. These experiments show that an intramolecular proton polarization gradient exists, except for EHBA where it coincides with the radius of its molecular structure. For EHBA-CrV the deuteration of the solvent was varied. In the absence of deuteration the radius of the radius of the magnetic spin diffusion barrier then appears to fall slightly below 5 Å, the radius of this molecule. Moreover, the characteristic times for the build-up polarized proton spin domains increase dramatically at lower concentrations of EHBA-CrV.

Molecular diffusion and hydrogen bond dynamics in liquid water at high pressure

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The complexity of the dynamics of liquid water results from the intermolecular potential which is dominated by very anisotropic hydrogen bonds. A rigorous approach must analyse the specific dynamics of hydrogen bonds which are at the origin of the unusual dependence of molecular dynamics on external conditions, temperature and pressure.

Quasi-elastic incoherent neutron scattering, because of its sensitivity to individual motions of hydrogen atoms, is one of the best tools to discriminate different components of atomic and molecular motions.

Early experiments on bulk supercooled water showed that the dependence of hydrogen bond lifetime on temperature is Arrhenius in contrast with the anomalous behaviour of transport properties [1].

For the first time, measurements were performed at 3 GPa and 400 K, in the region of melting of ice VII [2], using a new high pressure chamber [3]. They show: a) a strong decrease of molecular diffusion with pressure; b) a rotational diffusion, associated to the dynamics of hydrogen bonds, insensitive to pressure; c) the decoupling between temperature dependences of shear viscosity and translational diffusion at high pressure, thus the breakdown of the Stokes-Einstein relation.

Consequently, the decoupling of molecular (translational diffusion) and hydrogen bond (rotational diffusion) dynamics is observed also at very high pressures, a general feature resulting from the hydrogen bond network [4]. The breakdown of SE relation implies that extrapolation of molecular diffusion coefficients to pressures existing inside planets are not reliable. A best alternative consists to admit that the diffusion coefficient remains constant along the pressure melting line.

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Structural polymorphism in DNA-cationic liposome complexes: effect of composition, temperature and pH

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DNA polyanion interacts with a dispersion of cationic liposomes forming colloidal particles with organized microstructure, called lipoplexes. They attract attention as delivery vectors for genetic material. Despite the fact that cationic liposomes have been used for transfection, and commercial lipid formulations are available, their efficiency needs to be improved. Relationship between transfection efficiency, physico-chemical properties, their microstructure and polymorphic behaviour is still under discussion.

We will discuss structural polymorphism of two groups of lipoplexes prepared from neutral phospholipids with positive charges created either by gemini surfactants (CnGS12) or pH responsive N-alkyl-N,N-dimethylamine-N-oxides (CnNO). The binding capacity of complexes for DNA is in the range 30-95 % depending on the system and external conditions, as we derived from spectrophotometry. A small angle synchrotron X-ray diffraction (SAXD) was used to examine the microstructure of formed complexes. The surface charge density of cationic liposomes and the length of spacer of CnGS are key parameters modulating condensed lamellar (L_α^c) to inverted hexagonal (H_{II}^c) phase transition ($L_\alpha^c \rightarrow H_{II}^c$) observed in complexes with gemini surfactants. The *in vitro* transfection efficiency of CnGS12/DOPE lipoplexes in mammalian HEK 293 cell line is dependent on the CnGS12 spacer length. Structural polymorphism of the second group of complexes, with CnNO, is rich. In addition to L_α^c and H_{II}^c phases, we identified the presence of a cubic phase Q (Pn3m space group) at specific composition and temperature. Structural parameters of L_α^c phase, and the DNA-DNA distance are pH dependent. In this way, complexes prepared with CnNO represent pH responsive DNA nanocarriers. In the field of pharmacy, bicountinuos cubic phases attract attention as promising group of carriers for a large spectrum of drugs, genetic material (DNA, siRNA), small proteins or peptides including. .

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Magnetostriction of ferrogels and ferroelastomers

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Composite materials consisting of fine magnetic particles in the soft gels or relatively rigid elastomers are known as "ferrogels, ferroelastoemers, magentorheological gels/elastomers, soft magnetic elastomers". These systems present new kind of smart materials and attract considerable interest of investigators due to rich set of properties, valuable for many high industrial and bio-medical technologies (see [1,2] and references therein).

One of the most important, from the point of view of practical applications, and interesting, from the scientific viewpoint, problems of the physics of ferrogels and elastomers is the question on their magnetostriction (either elongation or contraction under the action of applied magnetic field). Some experiments and computer simulations demonstrate elongation of the samples in the field direction, whereas another ones – contraction of these systems (see, for example, [3-6]).

The type of this deformation is determined by the competition of the following factors. The first one is the change of the sample demagnetizing factor as a consequence of the sample shape variation. This factor stimulates elongation of any magnetizable media along the applied field. The second factor is change of the magnetic susceptibility of the material due to the variation of the mutual disposition of the particles after the sample deformation. This factor, depending on the structure of the particles spatial distribution in the matrix, stimulates either elongation or contraction of the sample in the field direction.

We present results of theoretical study of magnetodeformation of ferrogels with the linearly magentizable spherical particles. The following systems have been considered.

1. Composites with the homogeneous (gas- like) distribution of the particles in the polymer matrix. The results show that the type of the deformation depends on the shape of the sample and concentration of the particles. Initially strongly oblate or prolate samples must contract in the field direction, the samples of the intermediate shape – elongate. Analysis shows that increase of the particle concentration and appearance of the short-ranged order in their spatial disposition

stimulates elongation of the sample, increases the region of the sample shape, corresponding to the elongation.

2. The samples with the chain-like aggregates, parallel to the field direction. Analysis demonstrates the following. If gaps take place between the nearest particles in the chains, magnetic field induces contraction of the sample due to compression of the gaps. If, initially, the gaps are absent, the field elongates the sample due to specific of magnetic interaction between the chains.

Estimates show that magnetic interaction between the particles increases effective Young's modulus of the composites. This magnetoelastic effect must be especially significant for the systems with soft gel matrix.

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Oral Session

Upconversion luminescence of oxyfluoride glasses and glass ceramics

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Development of high-techs claims production of stable, energy-conserving and eco-friendly equipment. One of such techniques in optics is based on the upconversion effect. The basic ideas on upconversion were generated more more than 50 years ago in papers by Bloembergen and Auzel [1-2]. Later, for several decades this process, which is actually an anti-Stokes type of radiation, was widely studied by many authors and had several important applications among which are shortwave lasers, various opto-electronic devices, biophosphors, etc. To date the interest to the phenomenon of upconversion has received a new impulse due to the synthesis of modern matrix elements that contain various nanocomposites.

Novel composition transparent oxyfluoride silicate glasses and glass ceramics doped with Er^{3+} and co-doped with Er^{3+}/Yb^{3+} ions were synthesized. X-ray diffraction analysis (XRD) and Er^{3+} absorption spectra revealed precipitation of PbF_2 nanocrystals dispersed in the glassy matrix. Under 980 nm laser excitation, intense green, red and near IR bands of upconversion luminescence (UCL) were recorded both before and after heat treatment. Dramatic rise of UCL intensity by factor of ~ 150 was recorded for glass ceramic. To our knowledge, for the first time the composition of the glass ceramics characterized by the small-angle neutron scattering (SANS) showed the cluster organization of PbF_2 nanocrystals [3].

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Two magnetically soft microparticles inside an elastomer in an external field

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The magnetostatic forces between two micron size spherical particles made of an isotropic linearly polarizable magnetic substance and subjected to a uniform external field are studied. Under these conditions, the magnetization distribution within a given particle depends on the position and magnetization of the neighboring one.

The solution for the magnetic energy U of the pair has the form of power series with respect to the ratio of the particle radius to the particle center-to-center distance. The coefficients of this series are found numerically taking in about hundred terms. Evaluation of the interparticle forces, which requires differentiation of the energy over coordinates, is facilitated by proposing an approximate formula for U, which enables one to avoid the laborious numeric procedure. In such a way, the distribution of interparticle forces is obtained and compared to that provided by the point magnetic moment model. It is shown that at close neighboring of the particles, the magnetic force differs substantially from that predicted by the dipole model.

When analyzing the sign of the force, it is found that the angular interval between the field and the particle center-to-center vector, which corresponds to repulsion, is much more narrow than that for point dipoles. This means that in a system of magnetizable particles attraction is the dominating type of interaction.

The problem is extended to magnetomechanics by considering the same pair of particles in an elastic matrix. There, the state of the system, when magnetized, is determined by interplay of magnetic and elastic forces. It is shown that in the field applied along the center-to-center direction, the configuration of the pair essentially depends on the field strength. In a low field the equilibrium interparticle gap changes but slightly since weak magnetic attraction induces weak restoring elastic forces. However, in stronger fields the system becomes bistable: besides the energy minimum located close to the initial interparticle gap, another minimum emerges, which corresponds to a close approach (clustering) of the particles. In the latter state both the magnetic and elastic forces are strong.

Yet higher field eliminates the equilibrium at small deformation and the only stationary state of the particle pair is that of a cluster. Being not sensitive to thermal fluctuations, within the field strength interval of its bistabiliity the system behaves in a distinctively hystertic way.

This effect has important implications in mechanics of soft magnetic elastomers. In particlar, it explains the occurrence of "magnetic stapling" phenomenon, strong indications of which follow from experimental evidence.

Support by RFBR grants # 13-01-96056 and 14-02-96003), Ural Branch of RAS Programme #10 (12-P-01-1018) and project MIG S26/617 from Ministry of Education and Science of Perm Region is acknowledged.

Structural investigation of magnetic polydimetylsiloxane elastomers polymerized in different oriented magnetic fields

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Ferroelastomers were prepared using the radical polymerization of dimethylsiloxane with addition of ferrofluid based on magnetite. In the samples the concentration of magnetic component (ferrofluid) was varied: 1.27, 3.9, 5.88 and respectively 1.64 wt %. The magnetic field (B = 0, 280, 560, 1120 G) was applied perpendicular (Table 1) and (B = 0, 377, 1131 G) was applied parallel to the plane of polymeric film (thickness of ~0.5 mm). It was prepared also the polymeric matrix without ferroparticles (reference sample).

Tab.1 Samples $P_{32} - P_{35}$ synthesized in magnetic field parallel oriented to the elastomer surface [1,2].

Sample	Fe_3O_4, concentration, % mass.	Fe_3O_4, concentration, % vol.	Magnetic field induction B, 10^{-3}Tesla (Oe)	Magnetic field orientation
P_{32}	1.27	0.24	0	-
P_{33}	1.27	0.24	28 (280)	Perpendicular
P_{34}	1.27	0.24	56 (560)	Perpendicular
P_{35}	1.27	0.24	112 (1120)	Perpendicular

Tab.2 Samples $B_1 - B_4$, synthesized in magnetic field parallel oriented to the elastomer surface.

Sample	Fe_3O_4, concentration, % mass.	Fe_3O_4, concentration, % vol.	Magnetic field induction B, 10^{-3}Tesla (Oe)	Magnetic field orientation
B_1	-	-	0	-
B_2	1.64	0.31	0	Parallel
B_3	1.64	0.31	377	Parallel
B_4	1.64	0.31	1131	Parallel

The small angle neutron scattering experiments (SANS) have been carried out at ambient temperature (20°C) on the diffractometer "Membrane" (PNPI) in the range of momentum transfer $q = (4\pi/\lambda)\sin(\theta/2) = 0.03 - 0.8$ nm–1 where θ is scattering angle and $\lambda =$

0.3 nm is neutron wavelength ($\Delta\lambda/\lambda = 0.25$). In all the experiments there were studied the samples being isotropic in scattering plane. The incident beam was orthogonal to the planes of elastomers' films. Thus, the scattered intensities were dependent on the modulus q of scattering vector only. Since the neutron beam transmission for the samples was relatively high, Tr ~ 0.8, the multiple scattering processes can be neglected.

The scattering intensities are presented in Fig.1 and Fig.2.

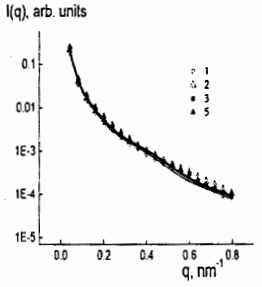

Fig.1 Scattering intensities I(q) vs. momentum transfer q for matrix P1(1) and ferroelastomers P32, P33, P35 (2), (3), (5).

Lines are approximation functions for matrix and ferroelastomers [1,2].

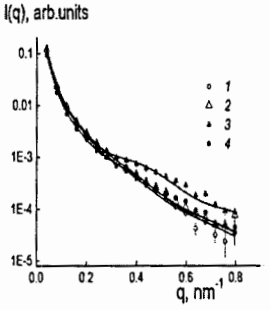

Fig.2 Scattering intensities I(q) vs. momentum transfer q for matrix B1 (1) and ferroelastomers B2, B3, B4 (2)-(4). Lines are approximation functions for matrix and ferroelastomers.

The best fit of the experimental data for elastomer matrix and magnetic elastomers polymerized in different oriented magnetic fields is obtained and discussed.

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FLNP JINR User programme at IBR-2 reactor after modernization

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The realization of the User Programme at FLNP JINR after IBR-2 modernization has been started in 2012. The spectrometer complex of the IBR-2 pulsed reactor at present consists of 11 instruments available for scientific research: 6 diffractometers, 1 small angle neutron scattering spectrometer, 2 reflectometers, 2 inelastic neutron scattering spectrometers. There are also 4 new facilities under realization: Diffractometer for studies of microsamples (DN-6), Multi-functional reflectometer with polarized neutrons (GRAINS), the new Neutron Imaging Instrument at the Beamline 14 of IBR-2 for radiography as well as tomography studies and finally the Fourier spectrometer for stress measurements.

Present state and the plan of development of a User Programme at Frank Laboratory of Neutron Physics, JINR are presented.

Small-angle neutron scattering studies of perfluorinated proton conducting membranes

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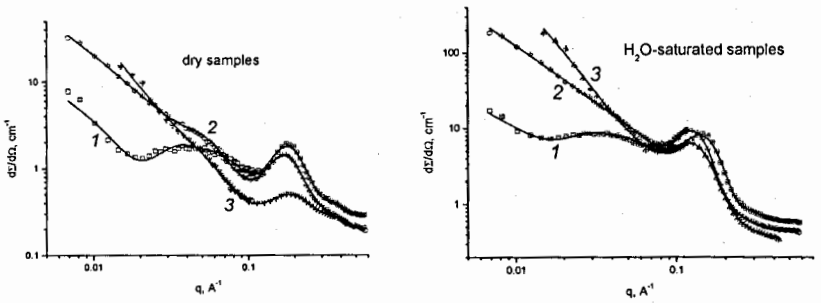
Fine structure features of long-side chain perfluorinated membranes was studied using small-angle neutron scattering. Membrane (*3*) produced according to new water-emulsion technique [1] was compared with Nafion® (*1*) and its Russian analogue (*2*), synthesized by traditional solution technique. New technique is characterized by a high productivity, reduced consumption of the expensive sulfonated monomer, and the possibility of controlling the equivalent weight of the resulting copolymer. Ionomer peaks at $q \sim 0.1 - 0.2$ Å^{-1} indicate strictly ordered structure, that can be described by correlations in arrangement of thin and long cylindrical channels (diameter is 9-14 Å in dry membranes and 20-25 Å in water-saturated samples). Nafion® has the most ordered structure, with straight parallel channels correlating on large distances (200 Å and more). Russian analogue of Nafion®, MF-4SK sample has a structure of curved channels. Scattering on PFM-E sample, obtained by new water-emulsion method, shows curved and branched channels, that can serve for more stable operation of the membrane and to improve proton conductivity through better interconnection of channels.

The preliminary studies of short-side chain membranes are also discussed.



1 – Nafion-115; *2* – MF-4SK, Russian analogue of Nafion®; *3* – PFM-E, membrane, synthesized by new water-emulsion technique.

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Magnetic properties investigation of a ferrofluid with cobalt ferrite nanoparticles using polarized muons

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A H_2O based ferrofluid with $CoFe_2O_4$ magnetic nanoparticles of 0.5% and 3% vol. concentration has been studied by μSR-metod. The measurement has been carried out in the temperature range of 26÷300 K in transverse to muon spin external magnetic field with the cooling of the sample in absence (ZFC) and in the presence (FC) external magnetic field.

It was found that regardless the mode of cooling in both samples the diamagnetic (muon) fraction formed in the ferrofluid is approximately in the same proportion as in H_2O. However, the relaxation rate and the precession frequency of the muon spin in the ferrofluid with 3% nanoparticles concentration depends on the cooling conditions of the sample, and they differ significantly from similar data for H_2O. The present results show that magnetic nanoparticles of cobalt ferrite have a high coefficient of magnetic anisotropy. The magnetic field created by single domain nanoparticles in ferrofluid has been found.

The work is performed in the Dzhelepov Laboratory of Nuclear Problems of JINR and the B.P. Konstantinov Petersburg Institute of Nuclear Physics.

Exchange integrals of commensurate and incommensurate structures of MFe_4Al_8 (M = U, Sc)

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The compounds with the general formula $M(FeAl)_{12}$ (M = Ac, Sc) crystallize in the body centred tetragonal system [1-4]. They form family showing a variety of magnetic structures, and in consequence of physical properties. In this lecture, we consider the origin of the complex magnetic ordering which deals with MFe_4Al_8 crystallizing in a tetragonal structure of $ThMn_{12}$ – type. The system of interest has four independent high-symmetry sites. The crystal structure of MFe_4Al_8 with I 4/mmm symmetry and cell parameters a~860 pm, c~500 pm contains: 2(a) – 4/mmm, occupied by M-metal, (8f) – 2/m – Fe site, and 8(j), 8(i) – m2m – tetragonal bipyramid formed around centring M by Al atoms.

In accordance with unpolarised single crystal neutron data UFe_4Al_8 exhibits commensurate magnetic ordering, i.e. $k_0 = \{0,0,0\}$ while $ScFe_4Al_8$ exhibits flat double modulated structure of the identical type of magnetic scattering vectors exhibits flat double modulated structure with magnetic scattering vectors: $k_1 = \{\tau_x, \tau_x, 0\}$ and $k_2 = \{-\tau_x, \tau_x, 0\}$, where $\tau_x = 0.13$ and 0.18 respectively [5]. Spin-canted system is realized in *ab*-plane with $\Delta\varphi = 0$ between iron spins along $[\bar{1}10]$ direction and with $\Delta\varphi \neq 0$ phase difference along$[110]$. The magnetic structure can be thought of as a superposition of two: non-collinear and collinear ferromagnetic lattices.

In order to construct a map of the exchange integrals reproducing the observed spin ordering, the atomic magnetic moments, modulation vector and phase transition temperature as well as diagrams of elastic neutron scattering the *MCMag* [6] and *MCPhase* [7] simulation programs were used. Both of them are basing on an algorithm of simulated cooling or heating, see Kirkpatrick [8], while the configuration space is examined by random sampling in accordance with the Metropolis procedure [9]. However, two crucial aspects make both methods different. While *MCPhase* allows finding the exchange integrals by means of a fitting (self-consistent Monte Carlo procedure) and treats the spins quantum-mechanically, much earlier developed *MCMag* treats the spins classically and the exchange constantans have to be guessed. Although the initial conditions and treated as the playing a

dominant role interactions in both simulation packages are different, both methods lead to a satisfactory description of the experimental results.

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Synthesis and magnetic properties of the multiferroic $GaFeO_3$ of orthorhombic and hexagonal symmetry

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This lecture is devoted to the multiferroic nature of gallium iron oxide. $GaFeO_3$ (GFO) has been intensively studied recently for its potential applications particularly as a magneto–electric material [1]. Such system can be used to switch its electric state vs. magnetic state and vice versa. Moreover GFO seems to be promising memory media which allowing a simultaneous reading and writing of data and will be useful in data storage as well [2]. The physical properties especially magnetism in $GaFeO_3$, depend strongly on the method of preparation. This work reports the preparation of $GaFeO_3$ by the sol–gel route (SG) and its characterization by x-ray and neutron diffraction as well as dc-magnetization and low and room temperature ^{57}Fe Mössbauer spectroscopy measurements. Many efforts have been expended on fabrication of gallium iron oxide by Pechini modification of the sol-gel method, which offers the possibility to synthetize multifunctional material. Moreover, the choice of SG synthesis was dictated by the possibility of obtaining the very small grains (~70 nm) [3]. According to a scenario using $Ga(NO_3)_3 \cdot 6H_2O$ [4] or dissolving metallic gallium in 10% solution of HNO_3 until to obtain the aqueous $Ga(NO_3)_3$ as a semiproduct reacts with a stoichiometric amount of $FeCl_3 \cdot 6H_2O$ in an environment of aqua distillate, citric acid (CA) and ethyl glycol (EG). The synthesis carried out in accordance with the standard procedure of SG where gallium nitrate (III) is a semiproduct allows obtaining single phase of the GFO with orthorhombic symmetry of $Pc2_1n$ space group, while the same procedure with the semiproduct of gallium chloride (III) leads to a single phase $GaFeO_3$ composition of corundum type - hexagonal symmetry of R-3c.The prepared samples are found to be single phase from x-ray diffraction studies. According to my best knowledge the perfectly ordered gallium iron oxide of an atomic ratio 1:1:3 is able to crystallize in an orthorhombic crystal structure only. Then the system forms a collinear antiferromagnetic ordering along [001] direction with the calculated magnetic moment of irons reaching up to the values of even $5\mu_B$ per atom [5]. Any disorder of the cations origin leads to more complicated non-collinear structures. So far for systems GFO the ferromagnetism [6], canted antyferromagnetyzm [7] or ferrimagnetism [8, 9] were reported. In the light of neutron diffraction and Mössbauer

measurements the strong correlation of the magnetic ordering against the cation distribution among the sites has been proven [10]. For example, as a result of site-disorder at orthorhombic as well as at hexagonal symmetry, the occupation of Ga^{3+} in one of the Fe sites alters the strength of the exchange interaction between Fe^{3+} ions by changing the Fe–O–Fe bond parameters and hence gives the possibility of tuning the magnetic transition temperatures and spontaneous magnetization values. Thus, the estimation of the cation distribution in each sublattice is necessary to understand the magnetic properties of $GaFeO_3$ system.

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Simulation of formation of chains in microferrogels using coarse-grained molecular dynamics

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Soft magnetically sensitive materials are composites with wide prospects consisting of polymeric gel carrier and nanogranular filler. The most intense trend in the intelligent materials science is the preparation and study of submicron-size isolated entities containing tens or hundreds of particles, in other words microferrogels [1]. They display tunable mechanical properties with respect to shape, density, and stiffness; moreover they are highly biocompatible. The main practical use for microgels is nanomedicine (or theranostics), where they enable immuno-probing and targeted drug delivery.

Effective practical implementations require adequate theoretical description of magneto-mechanical behavior of ferrogel samples. Molecular dynamics simulation provides a powerful and well-proven tool to study the response of microferrogels since it enables take into account a large number of structural units, whose motions and interactions determine the behavior of the ferrogel object. Dealing with microferrogels we need the coarse-grained modification of molecular dynamics. In such models, a group of molecules (or other elements) is treated as a single bead. This approach allows considering field-induced rearrangements of the nanoparticle's structures, which fundamentally determine the ferrogel magneto-mechanical response. We use the open-source software ESPResSo [2], which has already proven its efficiency in computer simulations of ferrohydrogels [3].

The microferrogel model is initially generated as a sample of a cubic lattice with 125 nodes. The nanoparticle sitting in each node site has a magnetic moment of a fixed magnitude and easy magnetization axis. The chains connecting the nodes consist of a number of non-magnetic particles interacting via hard-sphere and bonded potentials. First the sample is equilibrated at a finite temperature under a given intensity of steric and magnetic dipole interactions. Then a uniform field is imposed. We are interested in finding the main forms of the field-induced structural changes of microferrogel. Our results are presented with respect to the magnetic moment magnitude of particles, concentration of the magnetic grains and temperature. The presence of columnar structures in final equilibrium

configurations of small ferrogels because of the interparticle dipolar fields is clearly detected via radial distribution function.

Support by RFBR grants # 13-01-96056 and 14-02-96003, Ural Branch of RAS Programme #10 (12-P-01-108) and project MIG S26/617 from Ministry of Education and Science of Perm Region is acknowledged.

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Optical tweezers for studying of magnetic microparticles properties in liquid

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Magnetic microparticles have a variety of applications in biology, medicine and in the industry of magnetic devices [1]. Studying of the properties of magnetic fluids consisting of well-dispersed magnetic particles as well as applications of this fluids are rapidly growing. Magnetic forces between microparticles in liquid media are very small being in order of hundreds of femtonewton, so the ability to measure and control the forces is of considerable interest [2]. Also magnetic microparticles under action of external rotating magnetic field show complicated dynamical behaviour which is interesting from both fundamental and technological sides. Regarding the practical aspect, one of the most popular examples is a microvortex allowing to mix liquids on the microscales.

Application of optical tweezers enables to study properties of microobject without influence of substrate. It allows to control position of microparticle, detect they movement and measure forces and rotational moments acted on it [3].

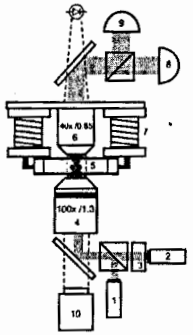

Fig. 1. 1, 2 – trapping lasers, 3 – acousto-optical deflector (AOD), 4, 6 – objectives, 5 – chamber with microparticles water suspension, 7 – electromagnets for magnetic field application, 8, 9 – quadrant photodiodes (QPD), 10 - CCD-camera.

In the present work the magnetic and mechanical properties of magnetic spherical microparticle are determined using optical tweezers technique.

Experimental sample was a water suspension of composite paramagnetic particles with a mean size of 3 μm made from polystyrene doped with magnetite (III). Fig.1 shows the setup of the double trap optical tweezers combined with external magnetic field system used in the experiments. Two optical traps were formed using laser beams of two diode lasers, which were focused using a high-numerical aperture objective. Two microparticles were trapped in optical traps at the fixed interparticle distance of L = 5.6 μm. The position of one of the traps could be dynamically moved in the sample plane using the acousto-optical deflector.

In the first part of experiment attractive and repulsive forces between particles were measured as a function of magnetic field and distance between particles. Suggested method based on nanometers displacement detection, it allows to measure weak magnetic forces accurate within few femtoNewtons and magnetic moment about 10^{-14} Am^2. This technique can be useful for micro scale magnetic properties characterization of particles suspensions used in medicine or technical devises.

In the second part of experiment microparticles rotation was achieved using external rotating magnetic field with frequencies from 1 to 100 Hz. Micriparticles rotation have a typical transition from uniform to non uniform rotation [4]. The frequency of transition between two modes depends on liquid media properties. This system was used as a microsensor for measurement of local temperature of liquid with volume about picolitters.

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Dynamics of magnetic microspheres under rotating field

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Magnetic microspheres with functionalized surface have plenty of applications, e.g. enable one to make fast quantitative detection of biomolecules directly in solution. With the aid of non-stationary magnetic fields, the microspheres could be set to motion becoming microtools for inter- and intracellular manipulations. In here, we study dynamics of microspheres under rotating magnetic field.

Let a microsphere be subjected to an external field $\boldsymbol{H}$ possess a magnetic moment

$$\boldsymbol{m} = \boldsymbol{m}_0 + \boldsymbol{m}_p = m_0 \boldsymbol{e} + \chi_0 \boldsymbol{H} + \chi_a (\boldsymbol{eH})\boldsymbol{e},$$

where m_0 is the permanent part, χ_0 и χ_a are the isotropic and anisotropic components of the paramagnetic susceptibility. Here for simplicity we assume that the microsphere anisotropy is determined by a single unit vector $\boldsymbol{e}$.

For the particle of submicron size, Brownian motion is an essential factor. An ensemble of such objects, provided their interactions are negligible, is described by a single-particle distribution function that obeys the rotary diffusion (Fokker-Planck) equation (FPE), see [1], for example.

Deriving from FPE the equations for the observable (ensemble-averaged) particle characteristics under a rotating field, one gets

$$\langle \boldsymbol{\Omega} \rangle = (\pi \eta d^3)^{-1} \langle \boldsymbol{m} \rangle \times \boldsymbol{H}, \qquad (1)$$

with $\boldsymbol{\Omega}$ being angular velocity of the particle, d its hydrodynamic diameter, and η the fluid viscosity.

Equation (1) has a clear physical meaning as it renders the balance of net torques acting on the particle. Analyzing it, one finds that there are two qualitatively different regimes of the particle rotation: (*i*) synchronous, where the particle follows the field under a constant angle lag constant, and (*ii*) asynchronous, where the particle angular velocity undergoes oscillations. Both regimes are observed experimentally [2].

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Field control over monolayer films of soft magnetic elastomers

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Elastomeric matrices filled with magnetic nano- or microparticles are known under several names: *magnetorheological elastomers*, *soft magnetic elastomers* (SMEs), *magnetoactive elastomers*, etc. None of them is exhaustively indicative since there are always a number of essential characteristics to be added: for instance, softness / rigidity of the matrix, magnetic softness / rigidity of the particles, their size, etc.

Nowadays, the most technologically prospective SMEs are weakly linked rubber-like materials filled with micron-size iron grains. These SMEs are rather soft rheologically and sufficiently loaded magnetically as to display considerable magnetomechanical effects like large field-induced strains, notable field tuning of the effective elastic modulus, certain type of shape-memory behavior and some other unique properties.

The most worked-on applications of SMEs' are field-controlled adaptable dampers and bearings. For those purposes, the bulk samples with all linear dimensions comparable: spheres, slabs, cubes, etc. are used. Our study is aimed at a different case, viz. the SME films. These quasi-two dimensional objects are more flexible mechanically and, thus, more sensitive to the applied field than the bulk ones. However, the macroscopic behavior of a SME film is, in fact, the net result of the particle-particle and particle-matrix interactions, both of which are 3D on the mesoscopic scale. Due to that, to get a correct description, a SME film is to be always treated as three-dimensional. To reveal the emerging specifics, we study here the magnetic field-induced deformations occurring in monolayer structures, i.e., SME layers with the thickness of the order of the particle diameter.

The response of such a film crucially depends on the direction of the applied field. An in-plane field arises deformations similar to that in a bulk sample except for the fact that the particles in the matrix have a reduced number of neighbors. Deformation of a film under a field normal to its surface is different. Magnetic softness of the particles ensures that all of them magnetize along the direction of the field. Meanwhile, as the film is monolayer, in the initial state there are no particle pairs, triades, etc. with the center-to center vectors parallel

to the field and, thus, making "head-to-tail" groups. Instead, all the particles are in the "side-by-side" positions relative to one another, so that their inter-center vectors lie in the plane of the film and perpendicular to the field. Given that the particle magnetic moments are parallel, in this situation the only type of magnetic interaction between the particles is repulsion.

Let the outer boundary (rim) of the film be fixed, thus making the film a membrane. For such a system, two mechanical response modes are conceivable. One is developing independently of the magnitude of the field. The mutual repulsion requires that the particles move to the positions, where they are mostly remote from one another. If no elastic forces existed, this would lead to a 2D triangle lattice. Having been initiated by application of a field, such self-regularization would stop at some stage due to the nonlinear growth of internal elastic stresses in the polymer matrix in response to the particle displacements. Evidently, provided the polymer is very soft and the particles are monodisperse, the process might rather closely approach the state of perfect lattice. This "in-plane" mode remains the only possible as long as the normal displacements on both faces of the film are forbidden. As mentioned, it has no threshold and develops in a field of any strength, whatever small.

For the situation, where the normal displacements are forbidden on one face of the film but allowed on the other, a new mode may develop. We note that from the viewpoint of the magnetic energy, the "head-to-tail" configuration of the particle magnetic moments is far more preferable than the "side-by-side" one. When one of the faces of the monolayer film is capable of distortions in the normal direction, a mesoscopic re-configuration of the particle structure becomes possible. For example, in a pair of particles which are neighbors in the plane of the film, one rolls atop of the other thus making the inter-center vector to turn about 90° and align with the field. To do that, one needs to spend energy $\varepsilon^{(\mathrm{meso})} \sim Ea^3$ per particle, where E is the elastic modulus of the matrix and a the particle size.

In a film with both faces free—let it be a membrane fixed by its rim—yet another mode emerges that is fully macroscopic, i.e., inherent to multi-particle systems. This shape instability of a SME membrane develops only after the strength of the imposed field exceeds a certain finite value. The symmetry considerations entailing appearance of a threshold are presented in [1], where this instability was considered in the framework of a continuum model. In the discrete formulation, i.e., in terms of the particle-matrix interactions/displacements, the mechanism is as follows.

Let a membrane subjected to a normal field, to form a "dome". As the surface of the dome (except the summit point) is inclined to the field direction, then the steeper the dome the greater is reduction of the magnetic energy due to the tilt of the interparticle center-to-center vectors. The elastic energy required for the onset of this deformation is $\varepsilon^{(\mathrm{macro})} \sim Ea^2/(nD^2)$ per particle, where n is concentration of the particles and D the size (e.g. diameter) of the membrane.

The mesoscopic modes inherent to the films with fully/partially immobilized surfaces are equally possible in a free membrane. However, comparing the elastic energy costs $\varepsilon^{(\mathrm{meso})}$ and $\varepsilon^{(\mathrm{macro})}$, one finds that the macroscopic deformation becomes preferable as soon as the particle concentration exceeds $n_* \sim 1/(aD^2)$. For the particle volume fraction this yields $\phi_* \sim (a/D)^2 \sim 10^{-6}$ that is very low with regard to any real MREs. In other words, a monolayer membrane of macroscopic size should respond to the imposed field by shape undulation, and under the fixed-rim condition, a single dome is the most long-wave perturbation of such a type.

The presented qualitative analysis facilitates understanding of the behavior of monolayer SME membranes obtained in our numerical experiments. The modeling is done on the basis of finite-element algorithm. A film with embedded spherical particles is considered as a continuum with piece-wise properties, where the particle substance is rigid and linearly magnetizable, while the matrix is a Mooney-Rivlin elastomer. By varying the boundary conditions, one is able to induce any of the predicted types of structure changes and to study each mode separately. By forbidding the normal displacements at both film surfaces, the undulation mode is excluded. Then, under the field increase, the in-plane particle distribution evolves from initially random towards the structure of a 2D triangle lattice. Setting free one of the surfaces, we observe the mesoscopic mode of structure changing, where some neighboring particles strive to get atop one another thus inducing at the free surface deformations with the wave vector $\sim a^{-1}$.

If only the rim of the membrane is fixed, the dome instability occurs as soon as the field strength exceeds a certain threshold value. Being very detailed, the numeric model enables us (*i*) to get the precise dome shapes as functions of the applied field and (*ii*) to observe and analyze how the mesoscopic spatial order changes in the assembly of the embedded particles evolve at the background of the large-scale perturbations (undulations) of the film.

The work is supported by RFBR grants #14-02-96003 and 13-01-96056, UB RAS Program #10 (12-P-01-108) and project MIG S26/617 from the Ministry of Education and Science of Perm Region.

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Poster Session

The structure properties of the chondroitin sulfate sodium salt from shark cartilage

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Chondroitin sulfate sodium salt from shark cartilage or chondroitin-6-sulfate (CS6) is a linear sulfated polysaccharide extracted from shark cartilage and is a major component of cartilage and joints. CS6 play an important role in osteoarthritis treatment, anticoagulant activity, reduces the degradation of cartilage matrix components, reduces necrosis and apoptosis of chondrocytes and reduces the activity of collagenase. Chondroitin sulfates are sulfated glycosaminoglycans that modify proteins in the extracellular matrix. Chondroitin sulfate is also responsible for proteoglycans degradation. Small-angle neutron scattering (SANS) measurements are made on dilute CS6 solutions to determine the structure properties of the CS6 chains. From the data we can see that increasing CS6 concentrations and calcium ion concentration, the radius of gyration increases. SANS data exhibit fractal behaviour and for them analyse the Beaucage and Broad Peak models were applied. In salt CS6 solutions SANS it can be observe the appearance of a correlation peak due to local ordering between adjacent chains in which the characteristic interchain distance is approximately 330Å. The increasing salt concentration the correlation peak becomes broader and weaker. From the data we can see that increasing calcium ion concentration, the radius of gyration increases.

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Influence of magnetic field and compression pressure on electrical conductivity of hybrid magnetorheological elastomers

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In this paper we have used graphene nanoparticles to fabricate a hybrid electro-conductive magnetorheological elastomer (MRE-hybrid). We manufactured a magnetoresistive sensor based on the MRE-hybrid and measured its electrical resistance in a transverse magnetic field (H), and separately, the electrical resistance under the influence of a compression pressure (p). We have determined the variation of electrical conductivity with H, and respectively with p and have developed a theoretical model which explains the effects of H and p on electrical conductivity of MRE-hybrid. The obtained results are presented and discussed.

[1] I. Bica, E. M. Anitas, M. Bunoiu, B. Vatzulik and I. Juganaru – "Hybrid magnetorheological elastomer: Influence of magnetic field and compression pressure on its electrical conductivity" – To be published, in Journal of Industrial and Engineering Chemistry.

High-conductive magnetic filler effect

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Material science plays one of the key roles in industrial growth. The invention and development of new machines formulates tasks for the designing of novel substances; on the other hand, the economy imposes the necessity to elaborate simpler and more universal technologies.

Also known as "smart", materials with controllable properties attract huge interest. Such areas as robotics, sensorics, electronics, machine construction etc. are potential users of devices and tools created on the basis of substances capable of quick and reversible wide-range changes in certain features caused by relatively small field or mechanical influences. Thus, owing to the prospects of this direction, this research has been dedicated to the studying of rubber-like composite magnetic composites with controllable electroconductivity as promising materials for sensors, dampers, and actuators.

Prepared by the impregnation of polymer matrix with thin carbonyl iron, such composites exhibit reversible magnetic field-dependences of rheological and electroconductive properties, for which the term "Magnetoactive elastomers" (MAE) has been attributed to them. This fascinating feature emerges owing to the phenomenon of magnetic filler structuring, i.e. the formation of chain-like structures oriented along the force lines by the particles, which results from both interaction between the magnetic dipoles with the external field and interaction among the dipoles. Thus, when placed in a field of 0.3T, a sample can exhibit a reduction of the electric resistance by 4-6 orders. At the same time, due to the elasticity of the polymer matrix, the formation of internal structures and such changes in the properties are fully reversible.

Among the problems encountered in the creation and investigation of MAE are the extension of the range of changes in their features and the stability of the materials with time. Owing to the fact that carbonyl iron is the most frequently used filler, corrosion is a factor responsible for the degrading of properties of interest initially reached in a sample. Attentive studying showed that it is also important to keep in mind initial surface corrosion of the iron powder, underestimation of which can be the reason why the product exhibits

conductive features noticeably worse than expected. Within the frames of the present research multiple experiments were conducted with the purpose to study the possibility to reduce the surface of somewhat oxidized iron particles as well as develop reliable methods of coating them with other metals having higher specific conductivities and exhibiting better resistance to corrosion.

Thus, our preliminary results give us the possibility to hope for success in the creation of universal devices of the extensive implementation area on the basis of MAE.

SANS investigation of $CoFe_2O_4$/lauric acid/DDC-Na/H_2O ferrofluid. Concentration effects

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Ferrofluids, ultrastable dispersions of magnetic nanoparticles in liquids, find a wide range of applications in many technical and industrial fields, as well as in medicine and biotechnology.

Cobalt ferrite nanoparticles ($CoFe_2O_4$) have received increasing attention for the combination of their bulk magnetic properties (high coercivity at room temperature, moderate saturation magnetization) with the magnetic properties typical of nanoparticles (superparamagnetism) that make them ideal materials for technological and medical applications.

In the paper results on concentration effects in a new non-ionic $CoFe_2O_4$/lauric acid/DDC-Na/H_2O ferrofluid investigated by means of small angle neutron scattering (SANS) are presented.

The ferrofluid was prepared by coprecipitation of $Fe(OH)_3$ and $Co(OH)_2$, ferritisation of hydroxide mixture in 1M alkali aqueous solution, adsorption of lauric acide on ferrite particles and peptisation of hydrophobic precipitate in aqueous solution with sodium n-dodecyl sulphate.

Small angle neutron scattering (SANS) experiments (Fig.1) were performed at the time-of-flight YuMO spectrometer in function at the high flux pulse IBR-2 reactor, JINR Dubna.

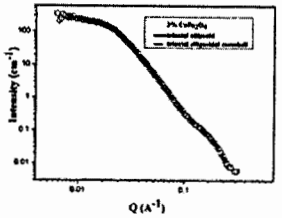
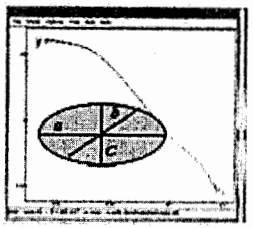


Fig.1 SANS experimental curve of 3% particle vol. concentration CoFe2O4/lauric acid/DDC-Na/H2O ferrofluid sample and model fitting.

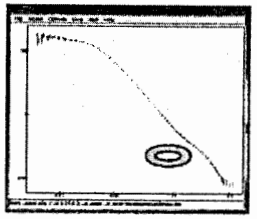
Using the FITTER package following preliminary results are obtained:

(i) for the range of 0.07 $Å^{-1} \leq Q \leq 0.8$ $Å^{-1}$ it is found for the form factor a triaxial ellipsoid model with half axes a, b, c:



a = (15.2±0.4)nm
b = (10.85±0.2)nm
c = (5.0±0.1)nm

(ii) for 0.8 Å-1≤ Q ≤0.3 Å-1 is determined a triaxial ellipsoidal shell model with half axes, a_{core}, b_{core},.c_{core} and shell thickness, t_{shell}:



a_{core} = (1.5±0.02)nm
b_{core} = (3.2±0.02)nm
c_{core} = (5.2±0.2)nm
t_{shell} = (3.3±0.1)nm

Nonthermal argon plasma generator and some potential applications

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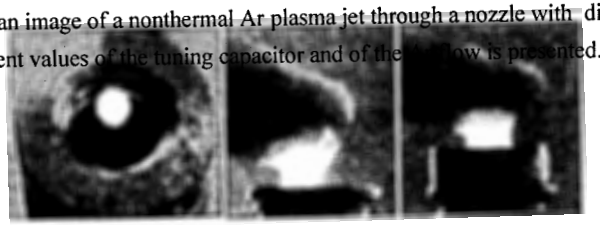
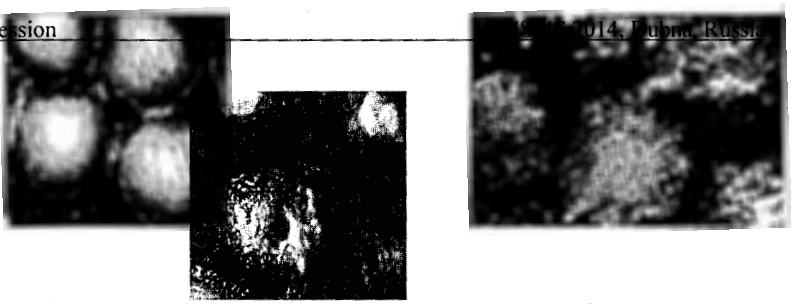
The plasma obtained by electric discharge can be either thermal, when the temperature of the electrons (T_e) is small compared to that of the ions or atoms (T_i), or non-thermal when $T_e >> T_i$. Both types of plasma are of interest for various applications. Thus, thermal plasma can be used for highly alloyed steels cutting and welding, tough and extra-tough semi-products splintering, or fine and ultra-fine powders production [1-4]. On the other hand, the non-thermal plasma can be used for biological environment decontamination [9], biocompatible surfaces preparation [10], cancer therapy [11] or gum and dental cavities treatment [12], etc., and the interest in nonthermal plasma has significantly increased during the last few years [7-14]. In all these applications (like in many others), an important role is played by the plasma generator; the present article proposes a non-thermal plasma generator as well as some results obtained in processing vegetal, biological and non-biological materials. In Fig.1 an image of a nonthermal Ar plasma jet through a nozzle with diameter of 0.01m for different values of the tuning capacitor and of the Ar flow is presented.



a) b) c)

Fig.1 Nonthermal Ar plasma jet through a nozzle with a diameter of 0.010 m, for different values of the tuning capacitor and of the Ar flow:
a) C=20 pF, g=0.00033m^3/s; b) C=240 pF and g=0.00033m^3/s, c) C=240 pF and g=0.00040m^3/s.

A leaf of *Anthurium andraeanumis* (Fig.2), samples of blood matrix, human hair and textile fibers were introduced in the plasma jet. For time periods of 30s and 60s, various effects like, cell detexturization, fast blood coagulation or textile fiber or hair cleaning and smoothing are obtained. These effects are presented and discussed in the paper.



a) b) c)

Fig.2 Foliage of Anthurium andraeanumis viewed with the optic microscope (magnification x20) unexposed in the plasma jet (a) and exposed in the plasma jet for 30 s (b) and 60 s respectively (c).

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Magnetorheological elastomer elasticity – based capacitor

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In the present paper, a magnetorheological elastomer (MRE) based on silicone rubber, magnetorheological suspension and catalyst, in a magnetic field, is obtained and studied.

The components used in obtaining the plane capacitor with MRE-based dielectric material are: silicone rubber, type RTV-3325 (Bluestar – Silicones), silicone oil (Merck), catalyst, 60R (Merck) and carbonyl iron (Sigma) as microparticles with diameter between 4.5 μm and 5.4 μm and iron content of min 97 %. A liquid mixture, consisting in 2.4 cm^3 carbonyl iron and 0.2 cm^3 silicone oil, is brought to the temperature of 573±5% [1] and maintained at this temperature for ≈ 5 minutes. At the end of the 5 minutes time the mixture is allowed to reach room temperature. Following the thermal decomposition of carbonyl iron, iron nanoparticles with average diameter of 61.2 nm are formed inside the liquid matrix [1]. The obtained product is mixed and homogenized with silicone rubber (1.2 cm^3±10%) and catalyst (0.2 cm^3±10%). The formed mixture is injected between two parallel copper plates (diameter 30 mm), provided on the outline with a spacer so as to maintain the distance between the plates at 3.5 mm±10%.The as-formed set was placed between the poles of a type Phylatex (Germany)-Weiss electromagnet. The magnetic field has a normal direction to the surface of the plane capacitor plates and intensity of H=840kA/m ±10%. After 24 hours, a plane capacitor with MRE dielectric material based on silicone rubber and iron nanoparticles (60% vol.) is obtained.

Using the plane capacitor method, it is shown that the elastic properties of the magnetorheological elastomer are influenced by the intensity and direction of the applied magnetic field.

The obtained experimental results are presented and discussed in the paper:

- The electric capacitance C of the plane capacitor with the MRE, the magnetic field – induced linear strain e and the stress σ depend on the strength and direction of $\vec{H}$;

- The magnetic Young modulus E of the MRE is strongly influenced by $\vec{H}$;
- The angle α between by $\vec{H}$ and the direction of the chains formed by iron particles decreases rapidly within the field range $20kA/m \le H \le 240\ kA/m$ and becomes constant for higher field values.

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Experimental study on fungi response to magnetic nanoparticles – antioxidant enzyme activity

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Laboratory simulation of magnetic contamination was carried out with focus on the cellulolytic fungi response to such external constraint. Nanoparticles of cobalt ferrite were prepared by chemical route being further stabilized with organic acid shell in deionized water at physiological pH. Diluted suspensions were designed to deliver to fungus cell culture magnetic nanoparticles concentrations comparable to literature reports data. Antioxidant enzymes were investigated through biochemical methods based on spectral data recorded in UV range from biological sample extracts. The results have shown the intensification of antioxidant enzyme production in the fungus mycelium as adaptation response to the increased level of oxygen reactive species resulted from the impact of magnetic nanoparticle supply.

Time-domain terahertz spectroscopy: a new tool for studying the Low-energy transfers in molecular crystals

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Inelastic neutron scattering (INS) spectroscopy used to be the most important tool in the studies of the low-energy vibrational transfers in molecular crystals which are strongly affected by intermolecular interactions. It also used to be the only vibrational spectroscopy method facing the terahertz frequency range. As entering the XXI century, there has been a tremendous activity in the field of basic and applied terahertz frequency research. A sizable fraction of this effort has been focused on the exploitation of the fact that most organic molecules in the solid state have a rich and distinct dielectric spectrum in the THz region, giving the most unique fingerprints.

Terahertz optical spectroscopy is only now beginning to make its transition from initial development by physicists and engineers (coupling the sub-picosecond laser pulses with high-end semiconductor devices) to broader use by chemists, with spectacular applicability in solid-state structural studies. The transition may be already found a great success as THz spectroscopy has the potential to provide a powerful and informative link between infrared spectroscopy and microwave spectroscopy, with potential in supramolecular chemistry, protein analysis as well as studies of molecular solids.

Here we present some examples of the time-domain terahertz spectroscopy studies of molecular crystals along with first-principles calculations, performed in frame of plane-wave density functional theory computations (DFT) in periodic boundary conditions, at the generalized gradient approximation (GGA) level.

The presented results underline the role of the numerical accuracy in the prediction of the lowest-energy phonon excitations in several hydrogen-bonded molecular solids.

Time-dependent density functional theory study on the electronic structure and spectral properties of some novel phtalimide derrivatives

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A lot of fluorescent organic compounds have found practical applications in science and technology as fluorescent molecular probes and labels. Among them, the best known are xanthenes, coumarins, naphthalimides, cyanines, various arylazoles, acridines and phenazines. Fluorescent probes are the most powerful tools that can be used for measurement of bulk solvent polarity or viscosity, as well as for monitoring changes of these properties in the probe surroundings, occurring at the molecular level. This is possible, because fluorescence characteristics of most of fluorescent probes is sensitive to the changes in solvation of the excited and ground states of the probe molecules, which in turn depends on the polarity and mobility of the molecules present in the probe surroundings. One important application of fluorescence probes is for monitoring progress of polymerization processes, especially photopolymerization. Since the first application of fluorescent probes for following progress of rapid photopolymerization processes, a lot of fluorescent probes suitable for monitoring free radical polymerization have been developed.

Here, we present the theoretical study of the recently synthesized family of phtalimide derrivatives, which were proved to be stable enough under heavy UV light exposure. Their good response and capability to accelerate the photopolymerization process makes them good candidates for practical applications in photocurable coatings industry.

The Time-Dependent Density Functional Theory (TD-DFT) has been applied in order to understand their absorption and emission properties. The potential energy surfaces were explored following the conformational and tautomeric space of the quoted systems in their ground- and excited-states. The performance of the several popular DFT functionals in the prediction of photo-physical properties was examined along with the influence of the solvent environment and polarity.

The performed computations have provided an interpretation of the recorded absorption and emission spectra allowing for understanding the nature of the related transitions.

Phase transitions of the PC membranes in the presence of the salts and sulfoxides

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The phase transition of the PC membranes is one of the more discussed questions in last years. It is well know that the temperature of the pre-transition (T_f) and main phase transition (T_f) depends on many external and internal conditions. For example, the extension of nonpolar lipids chains, external pressure, calcium ions, long alcohols and hydrocarbons increase the T_f.

In current work the influence of the salt and sulfoxides concentrations on the structure and phase transitions of the PC membranes was investigated by SANS at IBR-2, Dubna. It was shown that the temperature of the main phase transition increase with increasing calcium ions concentration ($C_{Ca^{2+}}$). The most significant effect was observed at low $C_{Ca^{2+}}$.

It was shown that sulfoxides such as dimethylsulphoxide (DMSO) and diethylsulfoxide (DESO) increase the T_f of the PC membranes. However, the phase transition occurs at lower temperature in the presence of the DMSO than in the case of the DESO at the same molar concentration of sulfoxides (χ_{DMSO}). Additionaly, we did not observe the transition of the fully hydrated PC membranes to the interdigitated phase in which hydrocarbon chains of one monolayer of the bilayer penetrate to the other in the case of the DESO at $\chi_{DESO} > 0.9$. The comparison of the effect of the DESO and DMSO influence on the membrane structural parameters and phase transition shows that DESO changes properties of lipid bilayers similarly but in a more 'soft' way than DMSO.

This work was supported by RFBR grant № 13-02-01460.

Anisotropic metal-polymer composites with spatially oriented mechanosynthesised FeGa particles

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Recent technological breakthroughs and the desire for new materials functions with decreasing working parts generate an enormous demand for novel materials. Composite materials can show superior properties compared with their pure counterparts. The ability of taking the advantage of particular properties of alloys particles as the constituent materials is the motivation for the development of metal-polymer functional composites. The present work has been undertaken to research the possibility of using mechanosynthesized intermetallic particles of bcc FeGa (galfenol) [1] in metal/polymer composite performance. We used particles of material that itself belongs to the class of high magnetostrictive materials. The presence of stresses in the particles due to mechano-chemical process of their preparation is a reinforcing factor in increasing their magnetomechanical effect. Recently it was reported [2] that intensive mechanical treatment of the bcc-iron particles in a planetary ball mill leads to the formation of particles with strain inducing magnetic anisotropy. It was shown that iron particles are crushed and flattened out in the elongated plate with the axis of easy magnetization oriented along the plane of flattening. We consider that this effect may affect the particles magnetostriction value by additional stress influence on the FeGa particle structure. So, all these effects: particles microstructure and their spatial arrangement in polymer matrix with suitable mechanical module should achieve the preferable anisotropy of magnetic characteristics with the aim to promote additional magnetomechanical response increase.

The preparation technique of the composite material had several steps [3]: 1) synthesis of particles with magnetostrictive phase composition by mechanical alloying of powdered Fe and Ga in an AGO-2 planetary mill, 2) filling of the liquid modified polyurethane with mechanosynthesised particles and ultrasound intermixing, 3) particles stabilization with orientation in polymer matrix applying external magnetic field .

Structure and magnetic properties anisotropy of developed composites have been carried out by scanning (FEI) and transmission (JEOL) electron microscopy, conversion electron Mossbauer spectroscopy, X-ray diffraction (Empyrean), dynamical mechanical analysis (Perkin Elmer), measurements of magnetomechanical and remanent magnetic anisotropy (JR-6, AGICO).

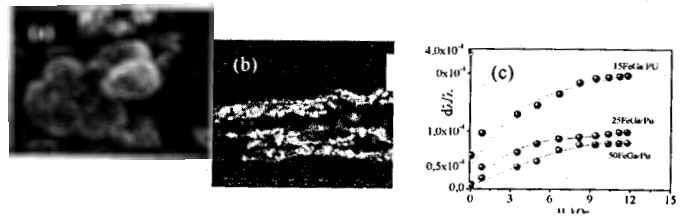

Figure 1. SEM images of mechanosynthesised FeGa particles (a), FeGa/PU composite (b), field dependences of magnetomechanical response via particle-to-polymer volume fraction (c)

Anisotropic chain structures of magnetic particles within the polymer with different interparticle interactions were observed [4]. The maximum values of functional characteristics were obtained for composition with 15% particles volume fraction with preferable spatial orientation of longest particles chains in field direction. Particles magnetostrictive phase composition induced lattice distortion and stress obtained mechanochemically posess the increase the own particles magnetostriction. Directed particles stabilization into associated chains enhances the magnetomechanical anisotropy of the composite.

Support by RFBR Grant 13-00-838 is acknowledged.

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Does the phase transition of lipidic membranes in nanodiscs exist?

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The paper presents the results of studying of phospholipid nanodiscs. In this work we researched the temperature dependence of nanodiscs geometrical dimensions using small-angle neutron scattering spectrometer YuMO (JINR, Dubna, Russia) [1,2]. The measurements were made for aqueous solutions of nanodiscs with compensation of protein density of the coherent scattering length (42% D_2O). The SANS curves were obtained for series of temperature points in the range from 22 to 26 °C. Changes of scattering curves in this temperature range are smaller then 3-sigma, where sigma is an instrumental error. These results are being discussed.

Acknowledgements: Russian Foundation for Basic Research (project 13-04-91320 and 13-02-01460), Russian program "5Top100" of the Ministry of Education and Science of the Russian Federation.

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Induced anisotropy of magnetic elastomers with low magnetic component concentration

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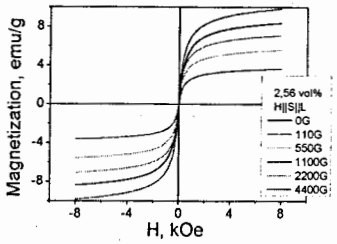

Fig. 1. The dependencies of specific magnetization on external magnetic field to MRE with 2.56 vol% magnetic particles in parallel direction to the plane and easy axis of the samples.

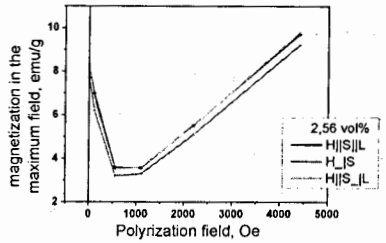

Fig. 2. The dependencies of the magnetization in the maximum external magnetic field on the polymerization field for different orientations with respect to the plane and easy axis of the samples.

The mechanical properties of magnetorheological elastomers (MRE) (elastic matrix based on magnetic particles) have been studied for several decades, but the electric and magnetic properties of MREs had got less attention. To study these properties of MREs there are important aspects of the structural features of the matrix (polymer type, polymer structure, etc.) and order/disorder arrangement of magnetic particles in the matrix.

In this study the MREs with low magnetic component percentage are investigated. Homogeneous mixture of dimethylsiloxane and ferrofluid with magnetite particles polymerized using catalysts. To induce the anisotropy in the samples, polymerization was carried out in a homogeneous external magnetic field (polymerization field). The samples were the sheets with thickness of 0.5-1.5 mm. Samples with concentration of 2.56 vol% of magnetic particles differ from each other in the polymerization field value (from 0 to 4400 G) that was applied in the parallel direction to the plane of the sample. As a result of polymerization field effect the preferred direction in the plane of the sample was easy axis.

Magnetic measurements were carried out with the vibration sample magnetometer "LakeShore" model 7407 at room temperature in the field range ±8kOe. The external magnetic field was applied in three directions to the plane of the sample: in parallel direction to the plane and to easy axis, in parallel direction to the plane and perpendicular to easy axis, in perpendicular direction to the plane of the sample. To prevent drying of the polymer matrix samples stores in polyethylene bags.

Typical dependences of specific magnetization on field are shown in Fig.1. These dependencies were unexpected - magnetization of various samples with same concentration differs by more than 2 times.

The dependence of the magnetization in the maximum field on the polymerization field is shown in Fig. 2. All three curves (different curves correspond to different geometries with respect to the plane and the easy axis of the sample) are nonmonotonic with a minimum at 500-1000 Gauss.

It is assumed that at high polymerization fields chains are formed in which the particles come into direct contact, as they form larger particles, which leads to magnetization increasing.

At low polymerization fields the magnetic moments of the particles are reoriented by the external field. As a result of dipole-dipole interaction between them, they repel each other, thereby particles are separated in the chain.

Thus the induced anisotropy as a result of polymerization field application was detected.

The work was financially supported by RFBR (grants № 13-02-12443, 13-02-90491).

Vibrational spectroscopy study of low-weight molecular crystals: the case of chloranilic acid complexes with α- and β-picolines

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Organic electronic materials including semiconductors, dielectrics and conducting polymers are emerging family of materials with applications similar to their inorganic counterparts, but of much greater potential ease of integration with silicon and other inorganic matrices. One of the most promising organic ferroelectric materials are built by two-component crystals formed by hydrogen donor and acceptor molecules. The family of chloranilic acid complexes reveals very promising properties which are extensively studied since last decade.

Here, we present the complementary structural and spectroscopic studies of novel chloranilic acid complexes with 2- and 3-methylpyridine, which were synthesized in our laboratory. The crystal structure for both systems was solved with single-crystal measurements. The optical vibrational spectra were recorded in the middle- (FT-IR; FT-RS) and low-frequency (FT-FIR, TDs-THz) range. The Inelastic Neutron Scattering (INS) studies were performed probing the low-energy transfers and revealing the closer insight into the vibrational proton-dynamics. The complex experimental studies have been deeply supported and interpreted by applying theoretical solid-state computations. The high-quality plane-wave density functional theory computations (DFT) were performed in periodic boundary conditions at the generalized gradient approximation (GGA) level. The lattice-dynamics has been probed with linear-response computations, providing both optical and neutron vibrational spectra. In addition to the Γ point computations, the phonon-dispersion relations and density of states were calculated across the high-symmetry points of the reciprocal space. The theoretical results stay in excellent agreement with the experimental data allowing for deeper understanding of the structural and vibrational properties of related molecular crystals.

The properties of a composition material "silicone rubber - particles of carbonyl iron"

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The elastic and anelastic properties of a composition material "silicone rubber - particles of carbonyl iron" were investigated by means of mechanical spectroscopy. The temperature dependences of internal friction (TDIF) and square of resonance frequency (TDf^2) of the composition material with the different content of the carbonyl iron particles (0 %, 35 %, 45 %) were measured in the range of temperatures from -50 to 200 °C.

Within this temperature interval the level of energy dissipation and elastic properties showed weak dependence on temperature. The imposition of a magnetic field of up to 2.5 A/m does not affect TDIF and TDf^2 samples with 0 % and 45 % of carbonyl iron particles. For the sample with 35% of particles the increase of the magnetic field leads to non-monotone change of an internal friction background.

The internal friction decreases with increasing of amplitude for samples with 0 % and 45 % of particles. The significant influence of a magnetic field on the amplitude dependence of internal friction of these samples was not observed.

Neutron and thermal analysis of new menthol derivatives

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The properties of a new series of thioesters: 4-(4-nonyloxybenzylothio) benzoates modified menthol (9OSBm), thymol (9OSBt) and carvacrol (9OSBc) are reported [1]. The chemical structure and purity of all substances were established with ^1H NMR, ^{13}C NMR and FT-IR spectroscopy. Mesomorphism was characterised with differential scanning calorimetry (DSC), polarizing optical microscopy (POM) and transmitted light intensity (TLI).

9OSBm exhibited polymorphism of crystalline phases. Replacement of the cyclohexyl ring of menthol part on an aromatic ring which is in 9OSBt and 9OSBc did not affect the appearance of the mesophases. All samples are stable and do not decompose after the transition to the isotropic phase.

In addition, study of the dynamics of selected functional groups for a basic substance which is menthol, using NERA spectrometer, operating at pulse reactor IBR-2 in Joint Institute for Nuclear Research in Dubna, was performed. What is more, for full vibrational characteristics of the functional groups of menthol, the infrared spectroscopy at the temperature range 20K - 300K was carried out. They were compared with the spectra generated using quantum-chemical methods. The equilibrium geometries, harmonic vibrational frequencies and infrared intensities for isolated molecule were computed using the density functional theory (DFT) with B3LYP functional. The basis sets used were 6-31G*, 6-31+G* and 6-311G**.

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Electronic, magnetic and transport properties in mesoscopic structures based on graphene

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The influence of size effects and chirality on the electronic, magnetic and transport properties of mesoscopic structures based on graphene are discussed. Graphene (the monolayer graphite) is a recently fabricated material consisting of an individual layer of carbon atoms arranged in a two dimensional hexagonal lattice [1-3]. There are two types of graphene structure, namely zigzag and armchair types. These structures differ according to their orientations and the directions of the edges. Electrons in graphene behave as 2D Dirac fermions and mimic the dynamics of hyper-relativistic electrons [4].

One shows that these properties of graphene are strongly dependent of their atomic structure edges and opens the way to the controllable onset of phase-coherent mesoscopic phenomena like quantum interference effects [5,6]. For this one resort to a tight-binding model Hamiltonian [7], which shows that graphene has full valence band and empty conduction band, while the top of the valence band has exactly the same energy as the bottom of the conduction band. Therefore graphene is called a zero band-gap semiconductor or semimetal, since electronic properties get ranged between the ones of metal and semiconductors.

We have described Aharonov-Bohm (AB) oscillations for the case of hexagonal graphene ring terminated in zigzag edges by means of an extended tight-binding model, now by using a single π-band [8]. The AB patterns characterizing the magnetization curves exhibit alternately integer (ϕ_0) and halved periods $(\phi_0/2)$, as long as the highest occupied state lies within the sixfold energy band. The $\phi_0/2$ period reflects the zigzag nature of underlying interior states [8-10]. The AB effect in graphene rings is a fundamental phenomena for quantum theory and it's important for applications in mesoscopic interferometric devices.

We investigated the evolution of the density of states (DOS) from graphene to a nanotube based on size quantization effects which arise as the dimensions are reduced[11].

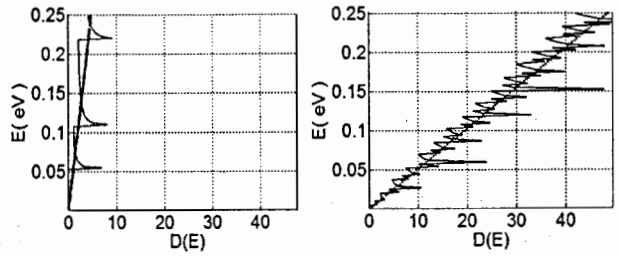

Figure 1. Density of states $D(E)$ for a zigzag nanotube (solid curves) compared with the one of graphite (crosses). (a) $m = 50$ (corresponding to $d = 3.85$ nm) (b) $m = 900$ ($d = 69.36$ nm).

It is obvious that in small nanotubes DOS is totally different from graphene, while in larger nanotubes this is less distinctive as shown in Fig.1, especially if we recall that experimental observations are typically convoluted with thermal broadening effects [11].

Those with small diameters have a large gap and those with large diameters have a small gap. This is especially true at high temperatures, when nanotubes with a large diameter begin to behave like graphene.

Aknowledgements. This study was supported by JINR-Romania, Scientific Projects, Topic no.04-4-1069-200912014, Protocol No. 4327-4-13/14.

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Dielectric relaxation processes in glycerol – glycine mixtures

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The work aims at investigating rotational dynamics of glycerol – glycine mixtures. Dielectric spectroscopy experiments have been performed in the frequency range (10^{-2} – 10^{7} [Hz]) and the temperature (173 – 303 [K]). The experiment has been performed for pure glycerol, pure glycine and their mixtures of various molar concentrations: (glycerol: glycine 1:2, 1:1 and 2:1).

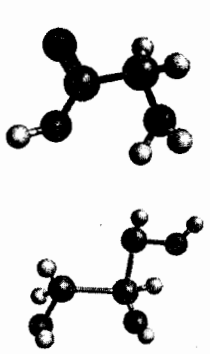

Fig. 1. The chemical structures of glycine (a) and glycerol (b).

It is known that dielectric spectra (ε") of glycerol exhibit (in the indicated frequency range) a single maximum [1,2]; our results well agree with the literature data. The dielectric contribution from pure glycine is negligible.

Comparing the dielectric spectra of glycerol in the presence of glycine with corresponding results for the pure solvent one sees for the mixture an additional relaxation contribution emerging on the low frequency side of the main relaxation peak. This contribution can be explained by slowing down of the rotational dynamics of a fraction of the solvent due to interactions with glycine molecules. The ratio of the magnitudes of the two relaxation processes observed for the mixtures is merely temperature independent.

The low frequency relaxation contribution indicates that a fraction of the solvent is slowed down due to the presence of glycine. Moreover, one also observes that the main relaxation peak somewhat shifts towards higher frequencies for large concentrations of the amino acid, which suggests that the rotational dynamics of the remaining (second) fraction of glycerol becomes somewhat faster.

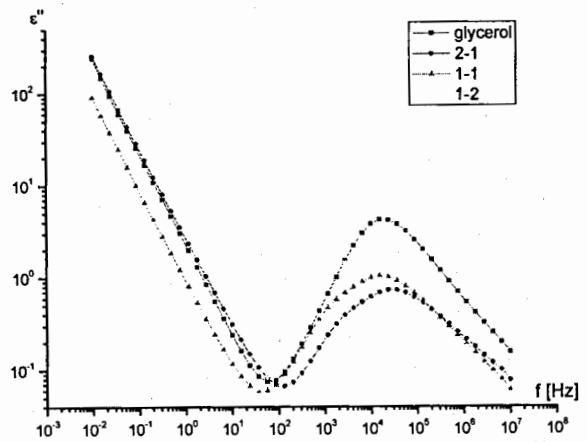

Fig. 2. The imaginary part of the dielectric spectra for a glycerol-glycine mixtures (all molar concentrations) and pure glycerol at 233 [K].

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2D Fractional Brownian motion simulation for the fractal properties of ferryhidrite nanoparticles.

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Small angle X-ray scattering (SAXS) offers valuable information on the size and morphology of the nanoobjects from the microstructure of the investigated samples. It enables measurements of structural features on a large scale interval $(1 \div 10^2)$ nm analyzing the scattering intensity pattern which is directly proportional to the size and shape of nanometer-sized objects.

For particular experimental situations, the scattering intensity profile for nanoparticles shows, for small values of the scattering vector Q, a power law dependence: $I(Q)=I_0Q^{\alpha}$, indicating a fractal nature of the structure. For $2<\alpha\leq3$, a mass fractal is defined with the fractal dimension $D_m=\alpha$ whereas for $\alpha>3$, a surface fractal with dimension $D_s=6-\alpha$ is defined. These values can be correlated with corresponding Hurst exponent $H=d+1-D$, where d is the dimension of the supporting space. If the Hurst exponent is different from 0.5, the surface is known as Brownian surface and it can be modeled as a 2D Brownian motion. For $H<0.5$, the situation corresponds to a fragmented surface with many small irregularities, while for $H>0.5$, is described a smoother surface.

Preliminary results on 2D fractional Brownian motion simulation for the possible structure configurations or aggregates that correspond to values of Hurst exponents identical with those computed from experimental power law dependence of SAXS scattering intensity from ferryhidrite nanoparticles samples are presented.

The fractal surfaces are generated using an algorithm based on Fast Fourier Transform (FFT) for stochastic power law noise characterized by specific Hurst exponent, summing all the terms in a 2D Fourier series, randomizing the phases and performing an inverse FFT [1].

A fractional Brownian surface is defined as a zero-mean Gaussian with nonstationary covariance function. The Hurst parameter characterizes the roughness of a random field.

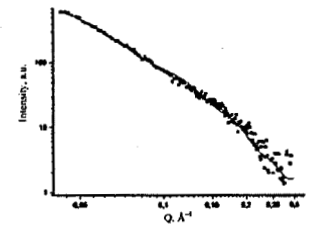

Fig.1 SAXS experimental curve for ferrihydrite nanoparticles dispersion in water [1].

For a relatively large range of the scattering vector Q, the experimental curves show a power low dependence, with exponent $\alpha = 1.73 \pm 0.01$ (Fig.1) [1].

This demonstrates that the scattering objects are a mass fractal with $D_m = 1.73 \pm 0.01$ for the situation presented in Fig.1. The simulated 2D fractional Brownian surface of the experimental result from Fig.1 corresponding to Hurst exponents $H = 0.26$ is presented in Fig.2.

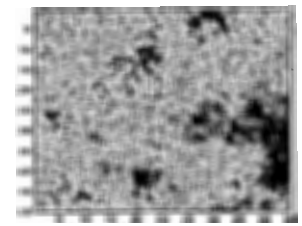

Fig.2 2D fractional Brownian motion that simulates the experimental result from Fig.1

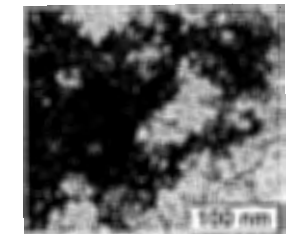

Fig.3 TEM image of a biogenic ferrihydrite water based dispersion sample

In Fig.3 a transmission electron microscopy (TEM) image of the same sample of biogenic ferrihydrite is displayed. The similarity between the two images can be interpreted as further evidence in support of our hypothesis on the importance of Brownian motion on the structuring of this type of ferrihydrite water dispersions.

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Biogenic nanoparticles of ferrihydrites

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Bayukov O.A.[2], Iskhakov R.S.[2], Antonov A.I.[1]

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Previously it has been shown that ferrihydrite nanoparticles synthesized by Klebsiella oxytoca bacteria in the biomineralization of iron salt solutions from the culture medium [1, 2] exhibit a unique magnetic properties: they are characterized by an antiferromagnetic order inherent in bulk ferrihydrite and spontaneous magnetic moment of the spins due to decompensation in nanoparticles sublattices. This paper presents the results showing that ferrihydrite nanoparticles are formed on the surface of the bacterial cell. The bacterial culture was grown in the Lovley medium, and then citrate buffer pH=5 (citric acid 40g / l, pH = 7 was set up by adding KOH) was added and further culture incubating during 1 to 25 hours was performed. The addition of citrate buffer in the culture medium did not significantly affects the number of viable bacterial cells in the medium, therefore, a citrate buffer does not destroys the cells. Upon the analysis of Mossbauer data we showed that after treatment of cell cultures with citrate buffer and washing the cells with the addition of NaCl there is no ferrihydrite nanoparticles in the suspension. This indicates that the nanoparticles were completely separated from bacterial cells. The above arguments lead to the conclusion that the ferrihydrite nanoparticles were synthesized on the cell surface of bacteria Klebsiella oxytoca.

Support by State Ministry of Education and Science is acknowledged.

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Magnetic resonance characteristics of biogenic magnetite

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Magnetite (Fe_3O_4) nanocrystals of biogenic origin are very interesting subjects of inquiry for magnetic resonance spectroscopy. At room temperatures (T=300K) magnetite is ferrimagnetic material with inverse spinel structure.

Presently there are some experimental facts of observation of electron magnetic resonance (EMR) signals of magnetite in biological systems. The wide anisotropic signals were detected in different biological systems: cultures of dividing cells, magnetotactic bacteria, organs of navigation and magnetoreception in insects, birds and fish, in mammal and human tissues (nerve, brain, heart, liver, placenta, blood etc.) in cancer cell cultures, in tumours. Up to now the nature of such signals is not quite clear despite of heated discussions.

In our research we investigated characteristics of EMR signals for the samples of human tumors [1] and nervous tissues in laboratory models [2]. Our research data and literature data allowed us to determine the following characteristics of the signals.

1) One or two line components with g-value higher than 2.1 of symmetric or asymmetric Lorentz shape (in different temperature intervals) are usually observed.

2) Characteristic non-monotonic temperature dependencies of resonance field (H_{res}), linewidth (ΔH) and integral intensity (I) with maximum for H_{res}, I and local minimum for ΔH near the temperatures 120-130 K is observed.

3) Anisotropic H_{res} behaviour of EMR signals was detected, which is character for ferrimagnetic resonance of magnetite crystals and which disappears near 130 K.

4) The correlations between the temperature dependence of the $H_{res}(T)$ and $\Delta H(T)$ and temperature dependence of magnetite magnetocrystalline constant $|K_1|$ are detected. To our opinion all the enumerated characteristics correspond to crystalline magnetite characteristics.

Sometimes wide EMR signals with g~5 and intensive zero field signals are observed.

Especially interesting is anisotropic behaviour of EMR magnetite signals. Angular dependencies of EMR signals were investigated in a wide interval of temperatures 100-200 K. The resonance field of EMR line is successfully described by the expression:

$$H_{res}(\theta) = \frac{\omega}{\gamma} - H_{ax}P_2(cos\theta) - H_{cub}\left[1 - \frac{5}{4}sin^2(2\theta) - \frac{5}{4}sin^4\theta\, sin^2(2\varphi)\right].$$

There are two contributions to the anisotropy of EMR line: axial and cubic anisotropy. Anisotropic parameters were found from the computer simulation of angular dependence of H_{res}, they changed with the temperature.

EMR anomalies within the interval 120-130K are evidently character to the Verwey phase transition in magnetite.

Detected EMR characteristics in different tissues and cells are similar to the characteristics of the signals in extracted DNA [3]. Coincidence of EMR characteristics for very different biologic systems allows us to suppose, that there is any universal phenomenon in all these cases and EMR is a perfect method of detection of biogenic magnetite and may become a new method of bio-medical diagnostics of storage iron in magnetite in biological systems.

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Polymeric nanocomposites containing metallacarborane: characterization by the means of small-angle X-ray and neutron scattering

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Globular micelles formation in water is usually observed with amphiphilic block copolymers, where the hydrophobic block is trying to avoid contact with water. Hereby we show the formation of particles for biomedical applications composed from 4-arm poly(ethylene oxide) - poly(2-methyl-2-oxazoline), (PEO-PMOX), and amphiphilic anion [3-cobalt(III) bis(1,2-dicarbollide)], (COSAN). Compounds based on boron clusters could be used for the treatment of a broad variety of biological targets including the inhibition of HIV protease, and others. Also, high content of boron allows using the composite for so called "boron neutron capture therapy (BNCT)" which is one of the most promising methods for cancer treatment [1]. In salted solution, PEO complexes with COSAN, which results in precipitation. This fact together with the weak interaction between COSAN and poly(methacrylic acid) was used to create core-shell particles of poly(ethylene oxide)-block-poly(methacrylic acid), (PEO-PMA), diblock copolymer [2]. The present complex with 4-arm PEO-PMOX copolymer does not produce such kind of structure, probably because of PMOX block interacts with COSAN. These interactions are weaker than that with PEO, which leads to formation of points with locally higher concentration of COSAN anions inside particle and results in characteristic peak at SAXS curves. The position of the peak corresponds to the distance between these points (~2.7 nm) and probably connected with the length of the blocks. SAS curves could be described with the form factor of sphere with Schultz-Zimm distribution of radius. The value of the radius is about 7 nm. The particle size distribution is narrower for the sample with higher ration of the COSAN content. Interestingly, the size of the particles remains the same in the wide range of COSAN concentration. A closer look on the behavior of two samples with the highest content of COSAN leads to the conclusion that copolymer particles have limited ability to store

COSAN inside. It is most likely that part of COSAN is located out of particles. It is valid for all the samples from these series due to the highly amphiphilic character of COSAN.

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Authors List

Information on Extreme Light Infrastructure - Nuclear Physics Project (ELI-NP) - Phase I

Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest, Romania
website: www.eli-np.ro

ELI-NP will be the Romanian research centre part of the European distributed infrastructure ELI. This will be based on two main pieces of research equipment, a laser system that will produce two 10PW beams, and a gamma beam system that will produce highly collimated, high intensity gamma radiation with tunable energy up to 20MeV. Due to the unique combination of these instruments worldwide, ELI-NP will be able to tackle a wide range of research topics in fundamental physics, nuclear physics and astrophysics, and also research that will soon find applications in materials science, management of nuclear materials, and life sciences. The project, valued at almost 300MEuro without VAT, received from the European Commission the approval for funding of the first phase (180MEuro) from Structural Funds (SOP IEC) and began implementation on the Măgurele Physics campus (near Bucharest). ELI-NP is to be completed and start operation in 2018 under an "open access" scheme.

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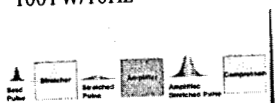

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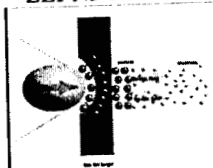

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• New ways of producing more efficiently radioisotopes currently used in medicine and the producing of newly proposed ones are also a promising research direction for the new

infrastructure. The intense neutron source at ELI-NP will find applications in the study of nanostructured systems, molecular and biomolecular physics.

Using at the same time both high intensity gamma and laser beams, the materials behaviour in extreme radiation conditions will be studied. This research is of high interest for, e.g., the production of components for nuclear power plants – the simulation of long functioning periods becoming possible.

• Another research topic very active at the moment is the acceleration of particles with the help of high-intensity laser beams. Different from techniques employed nowadays, using the classic particle accelerators, it has many advantages. Two of them are the much higher density (108 times with respect to an accelerator beam), relevant for medicine and materials science, and the width of the beam, that can be much larger and thus advantageous for hadron-therapy (in this modern therapy for certain types of cancer using protons or ions, the beam produced by classical accelerators must be scattered up to the desired width and thus potentially dangerous secondary neutrons are emitted).

• An area where ELI-NP will bring important contributions is the production with the help of the lasers of terahertz radiation – that lies in the frequency range beyond the possibilities of common electronics but below those of optical equipment. This radiation corresponds to rotation frequencies of large molecules and characteristic frequencies of some superconductors, and can be a powerful tool in many circumstances, such as: imaging of biological tissue, quality control in pharmaceutical and semiconductor industries, tomography in medicine, remote security screening. At the present time, this radiation is produced in synchrotrons and linear accelerators, which are very large and expensive equipment.

ELI-NP has the potential to be, for many years, in the fore-front of science worldwide, in several areas, from theoretical physics to biology. ELI-NP has a great flexibility to cover various interdisciplinary area, as a consequence of the possibility to employ simultaneously in experiments multiple radiation types, produced by equipment that will be unique at the moment of entering operation. The access to the infrastructure will be "open access" for not-for-profit organizations, researchers being able to submit proposals for experiments, then evaluated and selected by an international commission. Part of the operation time will be allocated to private companies that will pay the access costs, thus bringing a contribution to the ELI-NP operation costs.

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