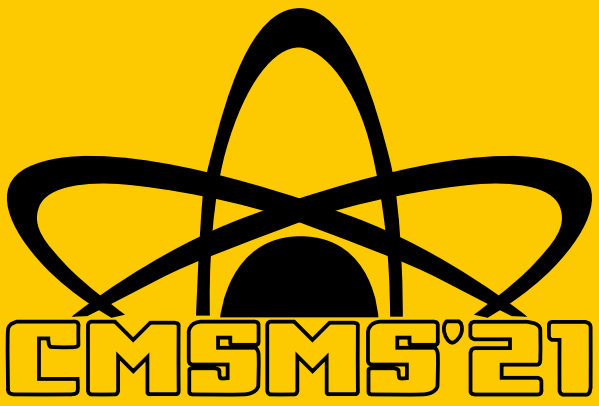

4th International Summer School and Workshop

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

19–22 April 2021, Timisoara, Romania

Book of Abstracts

JOINT INSTITUTE FOR NUCLEAR RESEARCH

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Preface

On behalf of the International Advisory Committee, Program and Local Organizing Committees, we welcome you to the virtual **4th International Summer School and Workshop on Complex and Magnetic Soft Matter Systems: Physico-Mechanical Properties and Structure (CMSMS'21).**

We would like to start by wishing you and your families our best—for your health and safety in these difficult times.

The COVID-19 pandemic has impacted many aspects of our lives. Following the recommendations on social distancing, and not wanting to postpone the event any longer, we moved the face-to-face meeting to a virtual one.

The CMSMS'21 is organized by the Joint Institute for Nuclear Research (Dubna), West University of Timisoara, Institute of Continuous Media Mechanics of the Russian Academy of Sciences (Perm), UNESCO Chair of the Belarusian National Technical University, Abdus Salam International Centre for Theoretical Physics, "Horia Hulubei" Institute of Physics and Nuclear Engineering (Bucharest), and Romanian Society of Physics.

Soft magnetic and complex matter topics encompass such fascinating materials as ferrofluids, magnetorheological fluids and polymers, magnetic colloids, ferrogels and magnetic and non-magnetic different nanoparticles, their associations with biomolecules and cells, other biocompounds and nanostructures and their applications. A highlight of this field is its large interdisciplinarity: this area has brought together scientists from condensed matter physics, theoretical physics, chemistry, and biology. While many of these systems have been investigated for a long period of time, only recently their common features have come into focus.

The aim of the CMSMS is to bring together both prominent scientists and students covering a broad range of scientific fields entering complex and magnetic soft matter systems research. The conference consists of invited talks, oral presentations, and posters. Some of the topics include: theory, simulations, and experimental research in physical, mechanical, structural, chemical, materials science, and 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.); aspects

of applied studies at large-scale research facilities, such as IBR-2, SOLARIS and others will be considered.

The workshop will provide a forum to share and discuss the latest advances for all active researchers in this field.

The First International Summer School and Workshop "Complex and Magnetic Soft Matter Systems: Physico-Mechanical Properties and Structure" (**CMSMS'12**) was organized by the Joint Institute for Nuclear Research (Dubna), West University of Timisoara, Institute of Continuous Media Mechanics of the Russian Academy of Sciences (Perm), "Horia Hulubei" Institute of Physics and Nuclear Engineering (Bucharest), and Romanian Society of Physics, and took place from 3 to 7 September 2012 in Alushta (Ukraine) at the JINR Spa Hotel. It 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 second event (**CMSMS'14**) was organized in Dubna from 29 September to 3 October 2014. It brought together 65 participants from Russia, Romania, Poland, Slovakia, Germany, and France. More than 10 invited speakers from Russian and foreign institutions provided a brief overview of several important research issues in complex and magnetic soft matter fields. Young scientists demonstrated a high level at both the poster session and the oral presentation. The programme included an excursion to the Frank Laboratory of Neutron Physics, where the participants visited the IBR-2 pulsed reactor and the IREN facility.

The third event (**CMSMS'17**), organized in Dubna from 28 to 30 June 2017, brought together 60 scientists from Azerbaijan, Belarus, Germany, Poland, Romania, Russia, and Slovakia. Fourteen invited lecturers delivered concise overviews of actual research issues in the school topics. Young scientists presented their results in oral talks. The poster sessions extended the frame of oral sessions providing opportunities for the scientific exchange in personal discussions to be continued. The presentations amounted to 35 contributions.

The main objective of **CMSMS'21, hosted by the West University of Timisoara,** is to exchange the latest research findings in the scope of the meeting. Around 90 pre-registered authors submitted their contributions. Young scientists were encouraged to present their results in oral talks.

The Organizing Committee is very grateful to the Romanian Plenipotentiary to JINR, to the Romania–JINR Cooperation Committee, to Frank Laboratory of Neutron Physics of JINR, and to the West University of Timisoara for the financial support of CMSMS'21. The conference received support under the RO–JINR Grant No. 267/20.05.2020, items 20, 33 and RO–JINR Projects No. 396/27.05.2019, item 44, No. 268/20.05.2020, items 29, 30, 31.

We express special gratitude to the West University of Timisoara Physics Department.

With all this, we hope that CMSMS'21 will be again a successful and stimulating scientific event.

Programme and Local Organizing Committees

INVITED

SPEAKERS

Ferrofluids at interfaces by neutron reflectometry

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The report reviews recent experiments on neutron reflectometry from ferrofluids at interfaces with solids. Study of the adsorption and arrangemnt of magnetic nanoparticles on solid surfaces is of current interest. In general, the dipole-dipole interaction between magnetic nanoparticles in ferrofluids enhances the layering of the particles on a planar surface. Still, the chemical interactions in the system affect much this process. It can be controlled by specular neutron reflection using a special design of the experiment when a flat neutron beam passes, meets and is reflected from the solid-liquid interface through a massive (here, single crystal silicon) block characterized by sufficiently high neutron transmission. The formation of the adsorbed layers of magnetic nanoparticles can be well seen in the reflectiviy curves interpreted in terms of the scattering length density distribuiton along the interfacae depth. The appearance and modifications of such layers were studied for ferrofluids based on different liquid carriers aimed at claryfying the effect of the structural stability in bulk on these processes [1-3]. The correlation with the formation of the adsorbed layers and aggregate state of the ferrofluids was analyzed. The research then were extended to the modification of the external conditions which affect the structural stability of ferrofluids in bulk. Thus, the effect of non-homogeneous magnetic fields (applied along the normal) on the particle assembly formation for a very stable ferrofluid was studied. At sufficiently high magnetic flux density, the enhancement of the layering was observed [4].

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Anisotropy of the elastic properties of magnetoactive elastomers

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Whereas some express the opinion that its role is so crucial that isotropic materials demonstrate little effect, others discern no difference between elastomers with and with no internal orientation. It has been noticed that magnetic elastomers polymerized under the influence of a magnetic field exhibit different elastic properties depending on the strain vector [1]. The present research has been dedicated to the elasticity anisotropy observed during stretching a strip of magnetic elastomer. Magnetic elastomers were synthesized by the conventional method assuming thorough mixing a magnetic filling powder with liquid silicone resin and vacuuming the suspension followed by distributing it on a glass plate and polymerization at an elevated temperature. As was found out from the following mechanical tests, application of a constant magnet causes a somewhat more pronounced effect; the following series of experiments were carried out using an electromagnet only. As the filling materials, there were used carbonyl iron powders, magnetite with cubic- and needle-shaped particles, iron fakes, mixtures of several magnetic powders. After polymerization in a magnetic field, MAE samples, containing carbonyl iron and γ-Fe_2O_3 particles, prepared in the form of a thin layer demonstrated structure formation as is shown in Fig1.

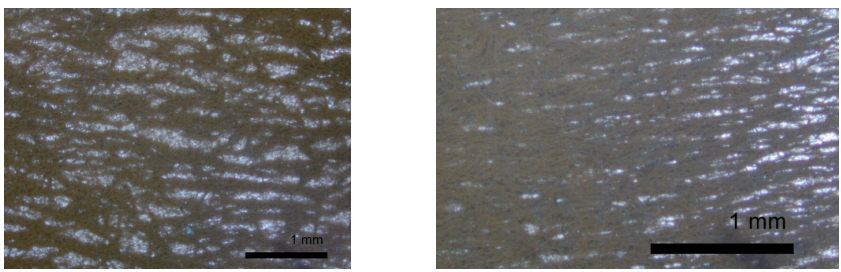

Fig. 1 Film structure of a magnetic elastomer

The samples were subsequently subjected to stretching in a pull test machine, during which their elasticities and strains at break were determined for two types of samples, namely cut from a strip in the direction parallel and perpendicular to the exterior magnetic field (as they are named in Fig. 2).

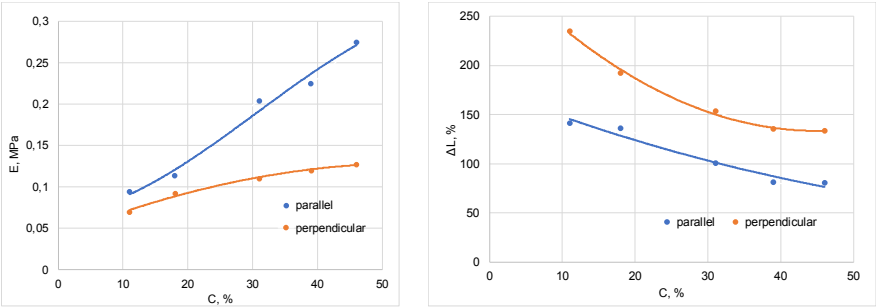

Fig. 2. Dependence of the elastic modulus at break of MAE on strain applied parallel and perpendicular to the magnetic field applied during polymerization

The obtained results suggest that samples stretched in a way parallel to the magnetic field used during polymerization exhibit a higher elasticity modulus in comparison to those cut out in a way perpendicular to the field. Thus, the elongations at break demonstrate opposite tendencies: samples stretched perpendicular to the magnetic field exhibit a higher elongation at break.

This investigation was carried out using samples with different concentrations of magnetic filler. Within the frames of this series of experiments, samples with high concentration were studied, because lower concentrations smooth out the effect. The fewer the magnetic particles are, the weaker the response of the sample is.

This phenomenon is determined by the specifics of the interior structure of magnetic elastomer, namely, by the distances between the particles and their agglomerates dispersed inside it. Along the direction parallel to the field used during preparation these distances are shorter in comparison to those separating particles in a perpendicular direction.

Financial support from the Russian Science Foundation (Grant #19-13-00340) and RFBR (Grant #19-53-12039) is gratefully acknowledged.

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Vibrating sensor element made of a magnetoactive elastomer

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The use of responsive materials, which characteristics can be significantly modified in a controlled way, is already providing the basis for many applications, including sensors and actuators. Among such devices are piezoelectric sensors [1], actuators with electroactive materials [2] and thermo-responsive grippers [3]. Magnetoactive elastomers (MAEs) form a special group of intelligent elastic compounds that exhibit a change in their shape and properties under the influence of applied magnetic fields. This is because they are made of magnetic microparticles embedded into a non-magnetic silicone matrix. Such a structure may therefore provide a wider technological application of MAEs compared to their liquid counterparts like ferrofluids and magnetorheological fluids [4,5].

This work focuses on the design and implementation of an MAE as functional vibrating element of an acceleration sensor. The proposed sensor system, as shown in Figure 1, consists of a straight beam, which is fixed to a housing at the top and made of an MAE with a concentration of 76.2 wt% of carbonyl iron powder. The beam is located inside of a cylindrical electromagnetic coil, the axis of which coincides with the beam's axis. Due to an external unidirectional excitation of the housing, the MAE beam displays in-plane bending vibrations. The key point is that the nearly vertical magnetic field generated in the inner area of the coil leads to a magnetisation of the MAE beam, which in turn changes considerably the vibration characteristics of the beam. Mostly, its basic eigenfrequency of transverse bending is the greater, the greater the current through the coil [6]. Experimental results of the steady-state response amplitudes show that the first eigenfrequency of the MAE beam is 8.95 Hz for a current of 0.5 A and 15.55 Hz for 2 A. This effect of the reversible tuning of the vibration characteristics is a basis for realisation of a variable sensitivity range.

The magnetic field in the inner area of the coil has also the second functional meaning. Its distortions caused by in-plane bending vibrations of the magnetised MAE beam can provide information to detect external mechanical excitation, e.g., acceleration [7]. The

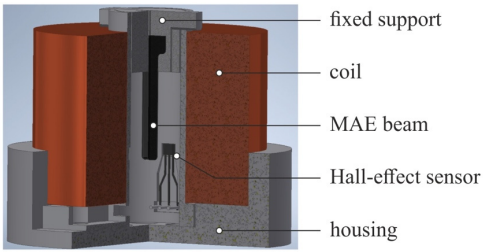

Figure 1. Prototype of an MAE-based vibrating sensor element

implemented field measurement strategy is to use two Hall-effect sensors that are fastened symmetrically to the inner tube of the housing at the height at which they can be touched by the end of the beam during its in-plane bending vibrations. Both sensors measure the horizontal components of the distorted magnetic field. The difference of these field values is the higher, the greater the deflection of the beam from its vertical equilibrium state.

Our prototype of the acceleration sensor with the MAE vibrating element is studied experimentally in response to a harmonic kinematic excitation of the housing and in the case of shock vibrations. The results are based on a comparison of applied excitations measured by a laser triangulation sensor with the field distortions recorded by the acquisition of the Hall sensor signals. It is shown that by changing the current in the coil, one can switch reversibly the configuration of the MAE vibrating element between the low/high frequency response and resonance response. For shock measurements, the applied acceleration peak value is proportional to the determined field distortion.

Financial support by the Deutsche Forschungsgemeinschaft (DFG) under the projects BE 6553/2-1 and ZI 540-17/3 is gratefully acknowledged.

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On the shear oscillating test of the magnetorheological elastomers

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Magnetorheological (MR) elastomers are composites based on an elastic polymer matrix and magnetic microparticles. The matrix of these composites usually is viscoelastic. It is expected that the presence of magnetic filler particles significantly changes the mechanical properties of the matrix. Furthermore, external stimuli, in particular magnetic fields, are used to control the viscoelastic response of MR elastomers. Thus, a correct quantitative characterization of the MR elastomer viscoelastic behavior under and without external magnetic field is one of the priority tasks in the field of MR technologies.

The most popular method for examining the viscoelastic response of MR elastomers is the shear oscillating test. In this test usually commercial rheometers are involved. The current talk addresses critical points related to the oscillating shear measurements, which are often ignored in experimental studies of MR composites as well as of even conventional unfilled elastomers. We compare different types of measuring techniques using a rheometer. Specimens of various geometries and compositions are used in order to critically evaluate the results obtained. Advantages and disadvantages of the rheometric oscillating shear test are outlined.

Financial support by Deutsche Forschungsgemeinschaft (DFG) under Grant No. Bo 3343/3-1 within PAK907 is gratefully acknowledged.

How chains and rings affect the dynamic magnetic susceptibility of a highly clustered ferrofluid

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The dynamic (frequency-dependent) magnetic susceptibility $\chi(\omega)$ in a highly clustered ferrofluid is studied using a combination of Brownian dynamics simulations and analytical theory. The particles are modeled as dipolar soft spheres, and magnetic relaxation occurs only through Brownian rotation with a timescale τ_B.

For ferrofluids with moderate dipolar coupling constants ($\lambda \leq 4$), the imaginary (out-of-phase) part of $\chi(\omega)$ shows a single peak at a frequency below $1/\tau_B$ due to the effects of interparticle interactions [1,2]. The focus of this new work is how chain and ring clusters affect the spectrum, and therefore a system at very low volume fraction (0.05%) and with $1 \leq \lambda \leq 8$ is studied. With $\lambda \leq 4$, the particles are not clustered, and $\chi(\omega)$ is of the aforementioned simple form. With $5 \leq \lambda < 7$, the particles form chains, and low-frequency features appear in $\chi(\omega)$, which are associated with chain rotation. With $\lambda \geq 7$, rings are the predominant structural motifs, and these give rise to new, high-frequency features in $\chi(\omega)$.

By analyzing an effective Langevin equation of motion for a single particle in the overdamped regime, the new, high-frequency features in $\chi(\omega)$ are shown to be due to motions of the particle dipole moments *within* ring clusters. Accompanying the structural progression, the static susceptibility $\chi(0)$ first increases, and then decreases, with increasing λ, and a classical density functional theory [3] describes and explains the trend very well.

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Non-equilibrium systems driven by particle rotation

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Behavior of systems with rotating particles (spinners, rollers) attracts interest from the point of view of active systems. Quincke rollers [1] and rotating membrane proteins [2] are just a few examples. An interesting system of this kind is described in [3] where it is shown that the ensemble of magnetic droplets rotating under the action of a rotating field forms a structure with hexagonal order. Here we describe a theoretical framework which may elucidate what is going on.

The rotating droplet is represented by the rotlet [4] which creates the velocity field

$$\vec{v}(\vec{r}) = \frac{\vec{M} \times \vec{r}}{8\pi\eta r^3}$$

where $\vec{M}$ is the torque acting on the droplet. The set of equations of motion of the droplets in the ensemble reads

$$\frac{d\vec{r}_i}{dt} = \sum_{i \neq j} \vec{v}(\vec{r}_i - \vec{r}_j)$$

Scaling the length with a radius of the droplet a and time by Ω the set of equations for the 2D case may be put in Hamiltonian form [5]

$$\dot{x}_i = \frac{\partial H}{\partial y_i};\ \dot{y}_i = -\frac{\partial H}{\partial x_i} \quad (1)$$

Set of Eqs.(1) has the integral

$$H = \frac{1}{2}\sum_{i \neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

Numerical simulation of Eqs.(1) shows that starting from some random configuration the ensemble of droplets remains in an disordered state (Fig.1a). It is important to remark that the rotational invariance of the Hamiltonian gives the second invariant [5]

$$\sum_i (x_i^2 + y_i^2)$$

which together with the conservation of the mass center position shows that the droplets remain at finite distances from the origin.

The behavior of the system changes considerably when the particles are made to repel each other. The formation of the ordered pattern when the droplet velocity due to the repulsive interaction between particles with the indices i and j

$$\vec{v}_{rep}(\vec{r}_i - \vec{r}_j) = \lambda_0(\vec{r}_i - \vec{r}_j) f(|\vec{r}_i - \vec{r}_j|)$$

where

$$f(r) = e^{(-\frac{r}{rs})}/r$$

is added is shown in Fig.1b. It is interesting to note that ordered structures may contain disclinations as shown in (Fig.2) and observed experimentally [3].

Research is founded by M-era-net project FMF No.1.1.1.5/ERANET/18/04.

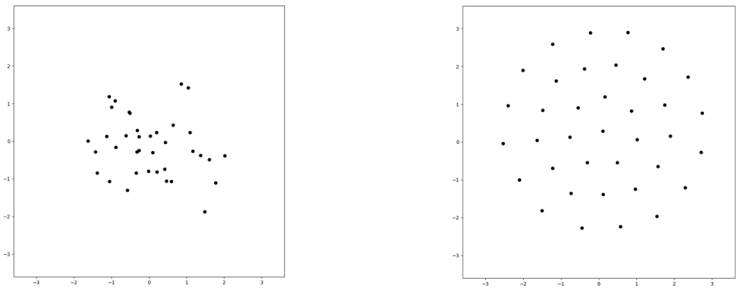

Fig.1. Particle ensemble at t=50 without (a, left) and with (b, right) particle repulsion starting from random state

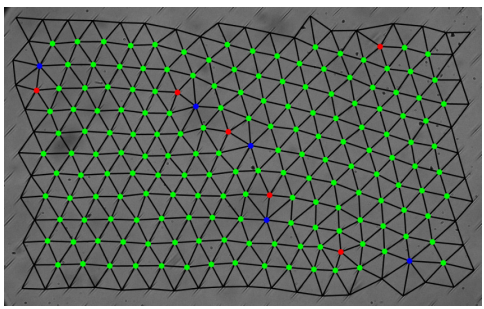

Fig.2.. Experimentally observed pattern of rotating magnetic droplets visualized by Delaunay triangulation. The dot color represents the number of neighbors in the lattice: red, green, blue correspond to 5, 6, 7, respectively.

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The influence of an AC magnetic field amplitude on the dynamic response of ferrofluid

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The investigation of the dynamic response of a ferrofluid on an AC magnetic field is of academic interest but also important for a number of applications. In diluted ferrofluids, where the dipolar interparticle interactions can be neglected, the dynamic theory is quite well developed for a wide range of AC field amplitudes. However, this theoretical approach is not sufficient when we deal with the high ferroparticle concentration where interparticle interactions play a key role. Many attempts have been made to include the effects of dipolar interactions to predict the dynamic response of ferrofluid (for instance, [1, 2]), but the obtained results can be applied only to weak AC fields. For a number of applications, however, the knowledge of the dynamic response in large AC fields is of vital importance. For example, in magnetic hyperthermia and magnetic particle imaging the ferroparticles are exposed to AC fields with a high amplitude. In the present work, a theory for the frequency-dependent magnetic susceptibility of a ferrofluid in an AC field with an arbitrary value of the amplitude is developed, including the dipolar interactions between the ferroparticles.

The ferrofluid is modelled as a suspension of spherical, uniformly magnetized particles. It is assumed that the relaxation of the magnetic moments of the ferroparticles occurs according to the Brownian mechanism. The rotational motion of a magnetic moment is described by the probability density which is the solution of the Fokker-Planck equation. The interparticle dipolar interactions are taking into account with the help of additional term into the Fokker-Plank equation. This term is determined on the base of the modified mean-field theory [2] in a systematic way, based on classical statistical mechanics. It describes the overall magnetic field produced by all other magnetic dipoles in addition to an AC magnetic field. The numerical solution of the Fokker-Planck equation is provided using the finite difference scheme with weights for convection-diffusion problems [3]. The probability density is used for the calculation of the real and imaginary part of the susceptibility. It is shown how various features of the susceptibility spectrum depend on the ferroparticle concentration, an AC magnetic field amplitude (Fig. 1), and intensity of

interparticle dipole-dipole interaction. Also, the dependence of the relaxation times of the magnetic moments on amplitudes of an AC field is studied.

On the basis of numerical calculations of the dynamic susceptibility, using the least squares method, simple analytical formulas were obtained for the real χ' and imaginary χ'' parts of the susceptibility of a ferrofluid depending on the amplitude α of the AC field and the Langevin susceptibility.

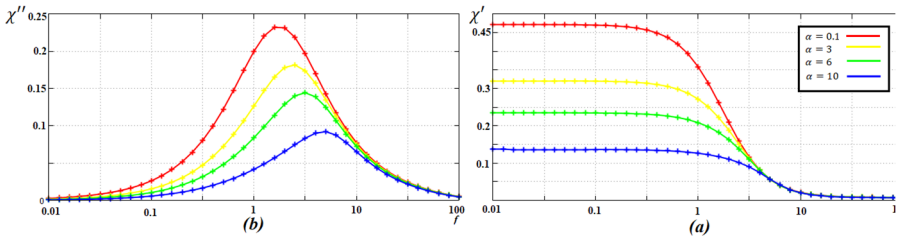

Figure 1. Imaginary (a) and real (b) parts of susceptibility versus reduced frequency f of the AC field for different field amplitudes a of the AC field. The Langevin susceptibility is χ_L=0.419.

The study was funded by RFBR, project number 20-02-00358.

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Collective relaxation times in the magnetization dynamics of Brownian magnetic nanoparticles

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Relaxation timescales in the magnetization dynamics of Brownian magnetic nanoparticles are studied using a combination of Brownian dynamics simulations and analytical theory, paying particular attention to the collective effect of the interparticle dipole-dipole interactions. The particles are modeled as dipolar soft spheres, and single-particle magnetic relaxation occurs only through Brownian rotation with a timescale τ_B. The collective time dependence is predicted analytically by solving the Fokker-Planck equation for the one-particle orientational distribution function. Interactions between particles are included by introducing an effective magnetic field acting on a given particle and arising from all of the other particles. Computer simulations are performed for monodisperse and bidisperse systems, and two different cases are studied. In the first case, the dynamic magnetic response of a ferrofluid to a weak AC magnetic field [1,2], and the frequency spectrum of the initial magnetic susceptibility, are calculated for various particle volume fractions and dipolar coupling constants. In the second case, the magnetization time decay under zero-field conditions, from an initially saturated state to zero magnetization at equilibrium, is investigated [3].

The main conclusion is that the effects of interactions are very significant. In each of the cases studied, the collective relaxation time of a moderately concentrated, weakly-interacting, monodisperse dipolar fluid is well described by the expression $\tau_{eff}=\tau_B\,[1+\chi_L/3]$, where χ_L stands for the ferrofluid Langevin susceptibility. Moreover, the effect of particle-size polydispersity is more pronounced for interacting particles, and the susceptibility spectra can be changed significantly by the influence of the collective interactions.

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Ways to tune self-assembly in magnetic soft matter

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In classical magnetic fluids with spherical polydisperse nanoparticles, dominating dipolar interactions typically limit structural complexity to linear arrangements. Those linear chains and branched structures are replaced by closed ring-like aggregates if the magnetic interactions grow or temperature is reduced. The structure and the number of aggregates can also be affected by tuning of the system granulometruc composition. These three parameters, *i.e.* temperature, granulometric composition and particle material, are not the only ones that can be used to control the microstructure of the magnetic soft matter. In this contribution I will show how a magnetostatic equilibrium state with noncollinear arrangement of the magnetic moments, as reported for ferromagnetic Janus particles, enables the controlled self-organization of diverse structures in two dimensions via constant and low-frequency external magnetic fields. Branched clusters of staggered chains, compact clusters, linear chains, and dispersed single particles can be formed and interconverted reversibly in a controlled way. The structural diversity is a consequence of both the inhomogeneity and the spatial extension of the magnetization distribution inside the particles. Next, I will discuss how after changing the carrier of the magnetic particles, one can exploit the competition between magnetic and elastic forces to direct the self-assembly.

Magnetoactive elastomers based on supersoft solvent-free bottlebrush polymer networks

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It is well established that the magnetic response of magnetoactive elastomers (MAEs) strongly depends on the degree of magnetic particle rearrangement in magnetic fields, which is mediated by an interplay of magnetic and elastic interactions. Softer polymer matrices allow for larger particle displacements in a magnetic field leading to a larger magnetorheological effect. Thus, the significant advancements in controlling viscoelastic behavior of MREs have traditionally been achieved by adding large quantities of silicone oil (up to 70 mass%) to soften the matrix. Liquid component is prone to leaching and thus significantly limits applicability of such materials. In this work, we report on the development of new solvent-free, yet supersoft MREs. They are prepared from polydimethylsiloxane (PDMS) bottlebrush macromolecules, i.e., polymers with densely grafted side chains (Fig.1). The brush-like architecture expands the diameter of the polymer chains, diluting their entanglements without markedly increasing stiffness.

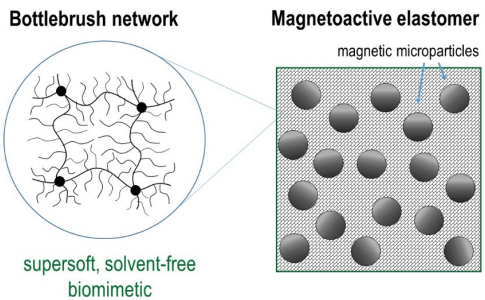

Fig.1. Schematic representation of a bottlebrush magnetoactive elastomer.

We demonstrated that combining two components (bottlebrush matrix and magnetic filler particles) is a synergistic tool for design of composites mimicking stress-strain behavior of various biological tissues. Bottlebrush architecture of the polymer matrix

allows to finely tune the material elastic modulus reducing it down to extremely low values while magnetic filler serves as an additional tool to control stress-strain behavior of MREs in a wide range of deformations including strain-stiffening. In the magnetic field, three orders of magnitude increase in the shear modulus of MREs was observed, which was accompanied by the material switching from a viscoelastic regime, characterized by values of the loss tangent, tanδ, close to unity, to an almost elastic one with tanδ close to zero. This level of viscoelasticity control can be obtained for MREs based on traditional linear PDMS matrices only by adding up to 70wt% of liquid plasticizer deteriorating MRE performance characteristics. The developed method for producing bottlebrush MREs by co-injection of components gives them additional advantages for biomedical applications.

Financial support from the Russian Science Foundation (Grant #19-13-00340) is gratefully acknowledged.

Revealing the interactions in conformational diseases modeling membranes by neutron scattering

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Alzheimer's disease (AD) is a conformational disease caused by the formation of senile plaques, consisting primarily of amyloid-beta peptides. The crucial role in this process at its pre-clinical stage is likely imparted by peptide-membrane interactions. The experimental data suggest several intriguing structural properties of biomimetic membranes that modulate such interactions. First, it is their sensitivity to the charge present in the surrounding environment. The structure of membranes changes for example with increasing concentration of ions, which appears to be an effect born by peculiar properties of ions and lipid themselves. Interestingly, the differences in lipid interactions with ions have been linked to the hydration properties of the ions. A plausible mechanism of action in the case of many membrane additives seems to be in shifting the water encroachment the way that bilayers absorb more or less water molecules. The hydration interactions appear to determine also the location of membrane constituents, such as cholesterol, melatonin, and amyloid-beta peptides. Moreover, cholesterol increases the order of lipid hydrocarbon chains while increasing the stiffness of membrane, in the contrary to the fluidizing effect of melatonin. The observations based on the neutron scattering experiments and MD simulations keep proving to be important for studies on amyloid toxicity and molecular mechanism of AD. For example, we have observed recently the changes in the membrane structural properties that were driven by the incorporation of amyloid-beta peptide to the system. During the temperature changes, the system experienced transitions between the vesicular and bicelle-like objects. The membrane shape changes were also accompanied by the dramatical changes in the membrane thickness. The conclusions of various investigations can thus provide an understanding for the possible structural changes taking place within biological membranes at the onset of AD.

Acknowledgement: This work has been supported by the Russian Science Foundation under grant 19-72-20186.

Small-angle neutron scattering at the pulsed reactor IBR-2: Nanoobjects and supramolecular structure study

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Structural studies play a key role in soft matter research, due mostly to the crystallography realized on synchrotron beam-lines. Small-angle neutron scattering on the other hand, is appealing to structural investigations of hydrogen-rich matter because of special features of neutrons. In particular, there are differing both the size and sign of scattering length density for hydrogen and deuterium that allow for employing the labeling and/or contrast variation methods.

Here we present some results and possibilities of the "YuMO" small-angle neutron scattering spectrometer (IBR-2, JINR, Dubna, Russia) [1], such as structural behavior of lipid membranes under different conditions (temperature, pressure, humidity), structural studies of complex nanoobjects and their additional components including proteins, DNA, various viruses [2], phycobiliproteins of the cyanobacterium Acaryochlorismarina [3] and other proteins.

Useful information about data treatment and experimental approach as well as examples using SANS facility for soft matter will be given [4-8].

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Diamond based nanostructures with metal-organic molecules

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Review of design, structural and physicochemical studies of nanostructures based on detonation Diamonds modified by metal-organic molecules to provide desirable functional properties (magnetic, fluorescent) has been presented. In these structures a mutual ordering of crystalline and molecular components was analyzed by neutron and synchrotron small angle scattering (SANS, SAXS). It delivered crucial information on subtle mechanisms of the interactions between organic molecules involving metal atoms (Diphthalocyanines, hydroxylated Endofullerenes captured Lanthanides) and Diamonds having positive surface potential in aqueous suspensions [1]. In aqueous solutions the optical absorption and X-ray luminescent properties of new objects are discussed regarding to their structure and composition relevant in biomedicine as effective contrasting agents in Magneto-Resonance Imaging (MRI) and photosensitizers in Photodynamic Therapy (PDT). We used expressly the Eu Diphthalocyanine (DPC) (Fig.1) with high photocatalytic and luminescent properties under UV and X-ray irradiation. The DPC molecules dissolved in dimethylformamide and transferred to aqueous dispersion of detonation Diamonds (DND Z+, 4.5 nm in size, ζ-potential ~ +(30-40)mV) form complexes with them (DPC fraction C_R = 0.1-1.0 % wt.), confirmed by optical absorption and dynamic light scattering. In water the complexes (DPC fraction C_R = 0.1-0.2 % wt.) created chain-like structures, but above critical DPC content C_R* ~ 0.3 % became highly ordered into branched structures by diamonds' linking via hydrophobic DPC molecules. Under X-ray irradiation the complexes with Eu atoms generated characteristic luminescence (wavelengths ~ 600-700 nm) that can be used for photosensitizers' excitation in PDT.

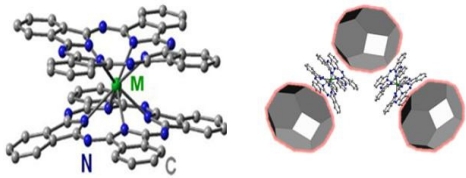

Fig.1. DPC molecule with metal atom (M) coordinated with ligands. Diamonds linking by DPC molecules with formation branched fractal structures.

These new materials may serve as catalysts for singlet oxygen generation in surrounding media (air, water, biological tissues) for cleaning, photoreactions' initiation, applications in recently developed X-ray induced photodynamic therapy (X-PDT). Further we used the Fullerenols $Gd@C_{82}(OH)_X$ (X~30) [2] to modify diamonds and create new structures with enhanced magneto-resonant and photodynamic properties. The formation of complexes of Fullerenols with DND Z+ was detected by UV-VIS absorption spectroscopy and small angle X-ray scattering (SAXS, Fig.2) showed subtle specific changes in SAXS-profiles.

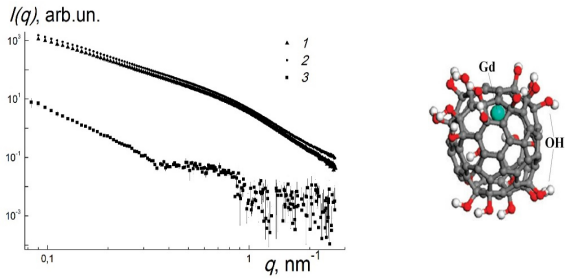

Fig.2. SAXS intensity (left) vs. scattering vector modulus for aqueous solutions of complexes (1), pure diamonds (2) and fullerenol molecules (3) shown also (right).

By NMR-measurements the associated Fullerenols comparative to free ones have induced 3-fold spin relaxation speed-up for protons in surrounding water that is really profitable in the creation of effective contrast agents for MRI-diagnostics.

The work was supported by the Russian Foundation for Basic Researches (gr. No 18-29-19008).

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Microwave magneto-permittivity of ferrofluids

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A theoretical model demonstrating the frequency (f) and magnetic polarizing field (H) dependence of the complex dielectric permittivity of ferrofluids ($\varepsilon = \varepsilon' - i\,\varepsilon''$) is presented. The theory is supported by measurements on a number of ferrofluid samples subjected to constant polarizing magnetic field, H, ranging from *0* up to the approximate value of *170* kAm^{-1}, over the frequency range *100 MHz– 6 GHz*.

The complex dielectric permittivity was measured using a *50* Ω coaxial cell, in conjunction with a network analyzer [1]. The polarizing magnetic field was applied perpendicular to the axis of symmetry of the measuring cell.

The experimental results show that the microwave permittivity of ferrofluids is determined by the Maxwell-Wagner-Sillars polarization phenomenon [2]. For well-stabilized ferrofluids, in which there are no particle agglomerations, the effect of H on the permittivity spectrum is explained by the rotation of particles with non-zero eccentricity and their alignment with the major axis parallel to the magnetic field. For ferrofluids in which there are large agglomerations of particles, the effect of H on the permittivity spectrum is interpreted in terms of spin valve effect [2], which manifests itself for adjacent particles inside the aggregates.

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The deformational response of magnetic gels and elastomers resolved from a mesoscopic scale

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Soft elastic materials, typically of polymeric origin, that contain rigid magnetic or magnetizable particles of colloidal size are frequently termed magnetic gels or elastomers, ferrogels or magnetorheological elastomers [1,2]. External magnetic fields induce magnetic interactions between the particulate inclusions, and via their mechanical coupling to the elastic environment, overall strains of the whole material can result. Thus, the use of magnetic gels and elastomers as soft magnetic actuators is conceivable.

In the present contribution, we investigate how the spatial organization of the particles influences the type of globally observed deformation. Linear elasticity and isotropy of the embedding elastic medium are assumed, while the role of compressibility is explicitly taken into account. Our studies are based on analytical calculations.

Altogether, we build on previous works, in which we had considered the magnetically induced configurational changes of particulate inclusions within an elastic bulk, far away from any system boundaries [3–6]. Displacements and rotations of the particles follow in response to the magnetically generated forces and torques. Our approach is confirmed by comparison with corresponding experimental examples [3,6].

To calculate the deformational behavior of a finite-sized system, the central challenge is to introduce explicit boundaries [7]. For the present purpose, we focus on the most accessible geometry at hand, namely, an elastic spherical body. We transfer previous analytical solutions for deformable spheres embedded in an infinitely extended elastic material [8] to free-standing elastic spheres [9]. The effect of the individual magnetizable particles is included by accordingly positioned force centers in the sphere. For simplicity, we assume all particles to be magnetized by a homogeneous external magnetic field to saturation. From the induced collective distortions and their evaluations on the surface of the sphere, statements on the overall types and degrees of deformation can be derived.

On this basis, we calculate explicitly the deformation profiles of the sphere when the embedded particles are organized in regular lattice patterns, or in a more randomized fashion [9]. We find that the internal particle arrangement has a quantitative and qualitative

effect on the type of deformation, for example, concerning changes in total volume, elongation or contraction along the field direction. In line with continuum theory and experiments [10,11], we observe that randomized particle configurations on average imply an elongation of the sphere along the external magnetic field. Changes of the compressibility can have a qualitative influence on the observed type of deformation.

Besides, we investigate the effect of incorporating initially twisted particle structures by the elastic sphere [12]. As a consequence, torsional deformations can systematically be initiated by magnetic fields. This suggests the fabrication of magnetoelastic twist actuators. Moreover, we analyze systems of binary particle size distributions [13]. It turns out that a targeted adjustment of the particle size within a given particle arrangement can reverse the type of overall deformation. Thus the particle size provides another parameter to tune the global behavior of the materials.

Altogether, we hope that our work will stimulate corresponding experimental developments and realizations to fully exploit the huge amount of degrees of freedom provided by the particle configuration in magnetic gels and elastomers. Accordingly, systems of optimized deformational response can be constructed. Especially, this requires the evolution of effective experimental methods to position a large number of particles in a continuous elastic medium in prescribed ways. An important advance towards the fabrication of materials of tailored magnetomechanical behavior will thus be achieved.

We acknowledge support of our work by the German Research Foundation (DFG) through the priority program SPP 1681 and through a Heisenberg Grant.

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Pseudogel of long-lived wormlike micelles and nanoclay particles

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Over the past few decades, there has been a great deal of interest in the aqueous self-assembly of surfactant molecules into giant wormlike micelles (WLMs). These cylindrical aggregates undergo reversible breakdown processes and in favorable cases can grow up to few tens of micrometers that is comparable with the length of high molecular weight polymer.

Rheometry, small-angle neutron scattering, and cryo-transmission electron microscopy were combined to investigate the structure and properties of mixed WLMs of zwitterionic oleylamidopropyl dimethyl betaine and anionic sodium dodecylsulfate surfactants. This system demonstrates the formation of giant linear long-lived WLMs, which even at extremely low surfactant concentration reach a sufficient length to entangle with each other and form a three-dimensional temporally persistent network. Stability of these micelles can be due to electrostatic attraction between the headgroups of the anionic and zwitterionic surfactants and favorable volume/length hydrophobic ratio in the surfactant mixture. Heating of these systems leads to the transition of temporally persistent network with predominantly elastic properties into transient network exhibiting viscoelasticity, which is due to the shortening of long-lived WLMs. At increasing surfactant concentration, the long-lived linear micelles transform into fast-breaking branched micelles, which is due to the screening of electrostatic interactions by salt released from the dissociated surfactant molecules. The transition results in the drop of viscosity and approaches the system to the behavior of Maxwell fluid with a single relaxation time.

Stable viscoelastic suspensions of bentonite clay particles in semi-dilute solutions of wormlike micelles of mixed surfactants were elaborated [1]. They represent a novel type of soft nanocomposite with tunable viscoelastic matrix. Structural studies revealed that the clay is dispersed in a dense network of entangled wormlike micelles in the form of 100-nm tactoids. Rheological investigations demonstrated that clay particles can induce an increase

of viscosity by up to one order of magnitude. The effect of the clay becomes more pronounced with increasing content of anionic surfactant in the mixture with zwitterionic surfactant, when the micelles become branched. This behavior was explained by the stabilization of micelle-nanoclay junction points due to the screening of the repulsion between positively charged fragments of zwitterionic head groups by added anionic surfactant. As a result of stabilization, the lifetime of surfactant-nanoclay junctions becomes much larger than the breaking time of micelles. The elaborated systems are of interest for many industrial applications.

This work was supported by the Russian Science Foundation (project № 17-13-01535).

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Can materials be smart? The fascination of magnetic hybrid materials

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The term "Smart Materials" has been used for many years both in scientific literature and in the press in general. This raises the question of what is meant by "smart materials"? If one looks at the literature here, it is generally assumed that these are materials whose properties can be altered by external stimuli. The number of possible stimuli is unbelievably large.

Ferrofluid under the effect of the magnetic field of a simple electromagnet

If one looks at materials whose influence can be technically used, magnetic hybrid materials represent a prototype of the "smart materials" class. These materials, which consist of magnetic nano- or microparticles in a non-magnetic matrix, can be controlled by the effect of magnetic fields.

If a simple Newtonian liquid is chosen as the matrix material, ferrofluids or magnetorheological fluids are obtained depending on whether magnetic nanoparticles or microparticles are used. The change in particle size alone leads to significant changes in material behavior in the magnetic field. While ferrofluids not only allow a change of their properties in the field but also an active magnetic flow control, magnetorheological fluids can be used to set a magnetically induced yield stress, e.g. for technically relevant force transmissions.

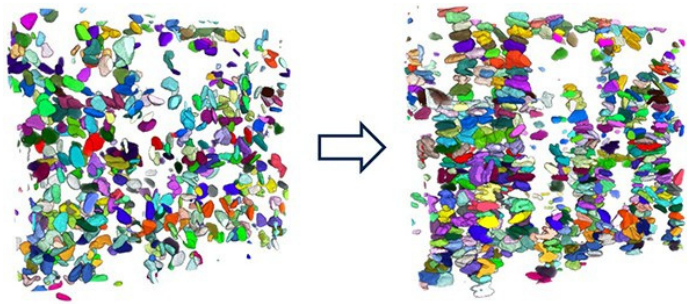
The possibility of influencing the material properties becomes even more extensive if more complex materials for the non-magnetic matrix are used instead of a simple Newtonian fluid. Liquid crystals, polymer solutions or blood can significantly expand the spectrum of liquid magnetic hybrid materials - even with a clearly application-relevant focus.

If elastomers or gels are used instead of fluid matrix materials, a new class of materials is generated that has been researched for about 15 years and is usually referred to as magnetic elastomers. In these materials, both the modulus of elasticity can be influenced

by magnetic fields and actuator deformations of the material can be induced. With these materials, too, the possibility of varying the magnetic as well as the non-magnetic component offers the opportunity to produce tailor-made materials for specific applications.

However, the targeted adjustment of material properties requires a detailed, cross-scale understanding of material behavior. At this point, variations in material behavior must be combined with microstructural changes, for which e.g. X-ray microtomography is an excellent tool.

In the context of the talk especially the use of X-ray microtomography for microstructural investigations and the link of such data to macroscopic properties will be discussed.



Magnetically induced magnetic formation of magnetic particles in a magnetic elastomer - made visible by X-ray microtomography.

Thermodiffusion of charged nanoparticles dispersed in EAN and water-EAN mixtures

Fiuza T.[1,2], Sarkar M.[1], Riedl J.[1], Repon G.[1,3], Cousin F.[4], Demouchy G. [1,3], Depeyrot J.[2], Dubois E.[1], Gélébart F.[1], Mériguet G.[1], Perzynski R.[1], Peyre V.[1]

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Ionic liquids (ILs) are a wide class of solvents, purely constituted of ions, which can be liquid at room temperature and thus strongly differ from classical molecular solvents. They are interesting for many applications due to their properties different from those of classical molecular solvents (very low volatility, versatility, and depending on the liquid, large electrochemical domain, wide temperature range….); For example in thermoelectric applications [1,2] that could then be operational up to a few 100°C.

Our work aims at developing new thermoelectric materials based on colloidal dispersions of maghemite nanoparticles (NPs) in IL solvents that are versatile, cost-effective and non-toxic to assist the economically and environmentally sustainable energy transition [3]. For catching the main parameters which rule colloidal stability and thermodiffusive properties of such ferrofluids (FFs), we present here a study in a well-known IL model system, Ethylammonium nitrate (EAN), miscible with water in any proportion [4,5]. Colloidal stability of FFs based on citrate-coated NPs in EAN and its aqueous mixtures is tested, together with the interparticle interaction, in a wide range of temperatures by Small Angle Scattering of neutrons or x-rays.

The thermodiffusive properties of these NPs are then determined with a Forced Rayleigh Scattering (FRS) technique [6,7] by inducing periodic thermal gradients in the light-absorbing NP's dispersions. In such ionic colloids, a gradient of temperature (∇T) induces a gradient of particles (∇n) thanks to the Ludwig-Soret effect (thermodiffusion), and a local electric field (E) thanks to the Seebeck effect (thermoelectric effect), both effects being strongly coupled [5,7,8,9]. The Soret coefficient (S_T) defined as ($\nabla n = - n\, S_T \nabla T$) is determined in stationary conditions, as well as the NP's mass diffusion coefficient (D_m) at the relaxation of the particle gradient, for various temperatures and concentrations.

In FF based on EAN, the ionic layering leads to a global interparticle interaction either repulsive or attractive, depending on nature of counterions and on water content. In water-EAN mixtures, thermodiffusion measurements show a non-monotonic evolution from the standard electrolyte behavior at low EAN fraction [8,9] towards that of the pure ionic liquid at large EAN fraction [5].

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Magnetic particles in an elastic environment: Variants of the magnetomechanical response

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Magnetoactive elastomers (MAE) with highly coercive fillers possess an extended, in comparison with usual MAEs, set of parameters by variation of which one is able to control the functionality (mechanical deformation, in particular) of these composites. This advantage is due to a possibility to impart to those MAEs a permanent magnetization by `initiating' them before use, viz. subjecting (and then withdrawing) a freshly prepared sample to/from a strong magnetic field. After such a treatment, the particles of NdFeB micron powder, which dwell inside the matrix until the end of polymerization in a demagnetized state, acquire substantial permanent magnetic moments.

A magnetic field applied to a sample acts directly only on the embedded particles, so that the magnetic control over the sample as a whole, i.e., the macroscopic magnetomechanics is entirely defined by the type and strength of the links between the particles and matrix and the character of emerging mechanical stresses. In usual MAEs, which are filled with low coercive (magnetically soft) particles, they mainly respond to an applied field by translational displacements of their centers of mass under the influence of magnetostatic multipole forces. In the MAEs whose particles are magnetized beforehand and keep their magnetic moments, not less important is the rotational mode (the particle centers of mass do not move) induced by the mesoscopic field-induced torques.

Until nowadays, for all the types of MAEs the question: to what extent of strength the particles are `glued' to the matrix still lies untouched and unanswered. In the meanwhile, in the modern MAE theory the assumption that the point-to-point contact at the particle/matrix interface is used by default, i.e., as a postulate, despite a lack of any justification.

In the present work, when considering MAEs with magnetically hard filler, we give physical grounds for two alternative models and discuss, whether it is possible to clarify the type of the particle/matrix coupling.

Model I [1] is specialized for real composites with NdFeB *Magnequench* particles of nearly spherical shape where the matrix is a silicon elastomer. As the estimates show, yet

under the fields about 1 kOe, the magnetic torque acting on the particles with diameter ~50 micron, is able to break the adhesion and `unleash' the particle from the matrix. Upon acquiring rotational freedom, the particle begins to rotate inside the cavity and stops only when the magnetic torque falls below the adhesion one. Each adhesion break adds some irreversibility to the magnetization process and affects the shape of the magnetization loop. Notably, the coercivity of such MAEs is in no way connected to the intrinsic properties of the particles and, thus, might be to an arbitrary extent lower that the coercivity of the particles themselves provided the latter is sufficiently high.

Model II [2] implies that the particles are non-spherical and, due to that, are congruent to the cavities which they occupy inside elastomer only in their initial positions. Besides that, we assume that particle/matrix adhesion is negligible in comparison with the particle Zeeman energy. This model, albeit it might seem not typical, has some unique features.

Under a field that is not parallel to the anisotropy axis of a given particle, the torque on the part of the field strives to rotate the particle that makes the latter to `shoulder' its way by perturbing the shape of the elastic cavity. The arising deformation of the matrix generates a resisting torque that impedes this displacement, and, thus, the urge of the magnetic moment to align with the applied field. A specific situation occurs, however, for the particles whose shape has some symmetry. For example, an ellipsoid-like particle has two magnetically different but geometrically identical states in its cavity. Because of that, the matrix resistance grows only until the angle of particle rotation does not exceed $\pi/2$. As soon as this border is trespassed, the torque produced by the matrix changes sign and now accelerates the particle in its fitting the cavity; on attaining the new state, the particle magnetic moment is inverted, i.e., the magnetization of the system is reversed.

We note that in the practice, the synthesized MAEs are filled with NdFeB of different brands, so that one may encounter, among other, either of the above-presented cases: a MAE with spherical particles (which are accounted for by model I) as well as a MAE with particles of irregular shape and low adhesion (for which model II is appropriate).

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Magnetoelectric effect in polymer-based nano- and microcomposites for biomedical applications

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Multiferroics is a class of material where magnetism and ferroelectricity interact. Coupled electrical polarization and magnetization give rise to their mutual control. For example, the direct magnetoelectric (ME) effect is the magnetically tunable polarization, change of the value or direction of electrical polarization under the applied magnetic field. Magnetorheological smart materials are a class of composite materials having both rheological and magnetic properties [1]. This kind of material is usually composed of ferro(i-)magnetic micro- or nanofiller and elastic polymer matrix [2]. One of the advantages of the elastic polymer composites is that they can be easily shaped for a specific application, for instance, via using a 3d-printer [3].

If the above properties (multiferroics and magnetorheological) are met in one continuity, these materials will merge attributes and advantages from both families. An interesting example is represented by the magnetoelectric polymeric composites — materials consisting of magnetic/magnetostrictive filler (e.g. magnetic nanoparticles) and piezopolymer matrix or polymer-bonded composites of ferroelectric and magnetic particles.

For this work, nanocomposites (NCs) were prepared based on polyvinylidene fluoride (PVDF) and its copolymer with trifluoroethylene (PVDF-TrFE). The aim of this work was to increase the coefficient of magnetoelectric transformation in polymer-based NCs suitable for biomedical applications (requests of low frequencies and biocompatible components and/or surface). For this, two new approaches to the creation of NCs were applied: i) ordering of magnetic nanoparticles in a matrix using a constant magnetic field and ii) modification of NCs with ferroelectric BaTiO3 particles. As a result of the experiment, the value of the magnetoelectric coefficient was increased from ~ 5 mV/cm·Oe for the composite of randomly distributed CoFe2O4 nanoparticles in PVDF

matrix to ~18.5 mV/cm·Oe for a composite of magnetic particles in PVDF-TrFE matrix with 5%wt of piezoelectric particles (Fig.1).

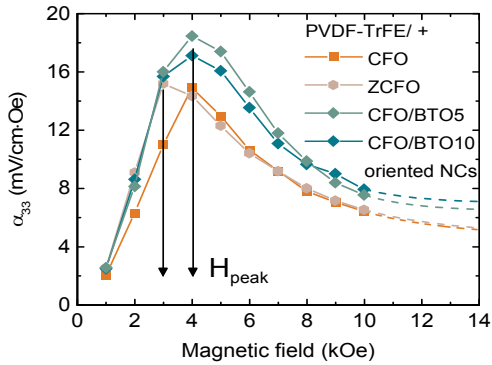

Fig. 1. Dependencies of the ME voltage coefficient (α_{ME}) on DC bias magnetic field composites at AC field frequency of 10 kHz for PVDF-TrFE -based samples with ZCFO, BTO5/CFO and BTO10/CFO fillers.

We tested the fabricated NCs for future use as biological interfaces for the activation of guided differentiation of neuronal stem cells. Neuronal stem cells cultured on the surface of PVDF substrates were able to proliferate and differentiate into the main types of nerve cells (neurons and glial cells).

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Microscopic modeling of magnetoactive elastomers

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A crucial simplification in most theoretical studies of magnetoactive elastomer (MAE) is the restriction to an exclusively linear magnetization behavior of the particle inclusions. However, in experiments often rather strong magnetic fields are applied where the linear behavior is no longer justified. Recently we developed a generalized formalism that provides a good approximation for low and intermediate field strengths and which is exact at large strengths in the saturation regime [1, 2]. The initial spatial distribution of particles and its change in an external magnetic field are considered. This is achieved by the introduction of an effective demagnetizing factor where not only the sample shape but also the MAE microstructure is taken into account.

The formalism allows to consider the non-linearly magnetized samples of realistic shapes like cylinders and cuboids. For example, the average magnetization in the axially symmetric samples, with the external field applied along the axis of symmetry, is compactly characterized by two factors. f_{macro} defines the demagnetizing factor of a sample along its axis of symmetry and f_{micro} is a scalar parameter describing the actual microstructure. Interestingly, the cylindrical and cuboidal samples exhibit a qualitatively similar macroscopic shape effect, compared to often studied spheroids. For the deformation and magnetization behavior of samples with stochastically isotropic particle distribution, a good agreement with explicit 2D micro-continuum mechanical modeling is demonstrated [3].

The generalized formalism allows us to calculate the stress induced by the external field in MAE samples fixed in a rheometer holder [2, 4]. The experiment is specially designed to access directly the influence of the sample aspect ratio in otherwise identical probes. This enables to separate the contribution of the macroscopic shape effect from the measured magnetic stress and thus to quantify the contribution from the microstructure effect. Clear trends for the isotropic and structured samples are established by fitting the theory predictions to the stress data measured in the experiment [2]. The samples prepared in the absence of magnetic field, and thus most likely containing microstructures close to isotropic, are characterized by the values of f_{micro} closer to zero. Contrary, the structured

samples prepared in the presence of magnetic field have a noticeably increased f_{micro} typical for chain-like structures.

The elongated microstructures are investigated recently in more detail on hand of helical chains with different angles between adjacent particles [5]. This allows to identify effects of local particle rearrangements in MAEs on their macroscopic behavior. Again, a remarkable agreement with explicit 3D micro-continuum modeling is observed.

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Magnetic anisotropy and particle-matrix coupling in soft elastic magnetic nanocomposites

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Dispersing magnetic particles in a nonmagnetic matrix enables the transmission of force and torque to the material without contact. In a mechanically soft environment, the propulsion of the magnetic inclusions entails elastic deformations, and such composites constitute a particular class of shape-programmable matter. The present study focused on two physical aspects which are crucial for the efficiency of torque-driven deformation of magnetic nanocomposites: the maximum torque associated with the anisotropy of magnetic nanoparticles and their local rotation in a soft elastic matrix. A microscopic model accounting for both factors was obtained from a detailed study of nickel nanorod/hydrogel composites.

The Ni nanorods, prepared by a template method [1, 2], are ferromagnetic single domain particles with uniaxial shape anisotropy, Figure 1. Their reversible magnetization properties could be well described by the Stoner-Wohlfarth (SW) model [3] after replacing the theoretical anisotropy constant K_A for an idealized homogenous spheroidal particle, as assumed in the SW-model, by an empirical model parameter. Exploiting the optical anisotropy of Ni nanorods enabled the detection of particle orientation and the investigation of particle-matrix interaction using polarized light optical transmission of dilute nanocomposites [4]. Ni nanorods, dispersed in soft elastic hydrogels revealed reversible rotation of the particle axis as function of magnetic field and orientation of the particle axis. The extended eSW model [4, 5], accounting for elastic particle rotation and the empirical anisotropy constant provided a quantitatively consistent description of the effective magnetic torque per particle as function of field and orientation. The torque density, derived from this microscopic eSW model, was implemented in a continuum calculation of macroscopic deformation and validated by comparison with experimental results.

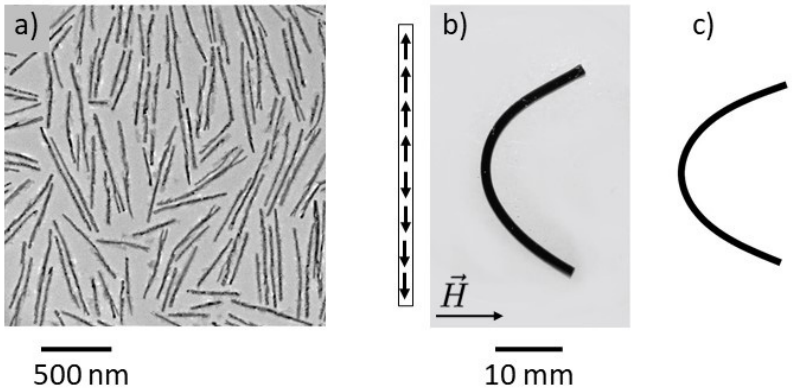

Figure 1: a) TEM image of Ni nanorods. b) Photographic image of a textured Ni nanorod/PAM filament in a homogeneous magnetic field of $\mu_0 H$=100 mT. For magnetic texturing, the nanorods were aligned parallel to the filament axis during polymerization and magnetized up/down in the upper/lower half of the filament, respectively. c) Computed bending profile with torque density obtained from the eSW model.

Thin filaments of textured Ni nanorod/polyacrylamide (PAM) hydrogel composites were prepared and the torque-driven bending and torsion in a homogeneous magnetic field measured, Figure 1b. The comparison with model calculations, Figure 1c, provided detailed information on the microscopic state of the magnetic nanoparticles inside the deformed composite. The contribution of finite magnetic anisotropy and local elastic rotation was found to vary significantly, depending on experimental conditions, e.g., the nanorod volume fraction or the elastic modulus of the filament matrix material.

Irreversible switching of the magnetization in opposite direction reverts the direction of the local torque which may be detrimental and requires proper design of the magnetic texture. On the other hand, such magnetization reversal allowed a re-programming of the field-dependent shape profile.

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Structural changes of pulmonary surfactant induced by endotoxin and Polymyxin B: SAXS and SANS

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Pulmonary surfactant (PS) lines the interior of the lung alveoli and acts to lower the surface tension at air-liquid interface. PS is composed of lipids (~90 %) and ~10 % specific surfactant associated proteins. The absence of PS due to prematurity, or its damage, is treated by exogenous PS in neonatal medicine. Curosurf (Cur), clinically used exogenous PS extracted from porcine lung tissue consists of phospholipids and a small amount of the essential SP-B and SP-C proteins (~2 %). The hydrophobic protein SP-B generates oligo- and multi- lamellar organization of Cur. We determined structural parameters of Cur, the repeat distance d and the thickness of lipid bilayer d_L, combining techniques of small angle X-ray and neutron scattering (SAXS and SANS).

Bacterial endotoxin, lipopolysaccharide (LPS), is the major component of the outer membrane of Gram-negative bacteria. In the lungs LPS interferes with PS resulting in its inactivation. Molecules of LPS interact with lipid bilayer of Cur and disturb its multi-lamellar structure by swelling as revealed from SAXS. The observed structural changes were attributed to the surface charge unbalance of the lipid bilayers due to LPS insertion. Alongside, LPS prevents the exogeneous PS from reaching the necessary low surface tension (γmin) during area compression, mimicking the respiratory cycle in pulsating bubble surfactometer [1].

Polymyxin B (PxB) is an antimicrobial decapeptide primarily used in clinical practice to treat infections by resistant Gram-negative bacteria. Recent experiments have shown the restoration of PS activity by PxB in LPS potentiated injury of immature rabbit lungs [2]. Our SANS experiments have shown that PxB facilitates fusion of unilamellar Cur vesicles with a slight decrease in the lipid bilayer thickness d_L. Model system of PS prepared from a mixture of lipids (DPPC/POPC/PLPC/POPG) has shown similar behaviour. PxB acts as an inhibitor of structural disarrangement induced by LPS and restores original multi-lamellar packing as confirmed by SAXS. Alongside with structural restoration of the

LPS/Cur system, the surface activity improved with increasing PxB concentration, as detected by the decrease in γmin [1].

Our SAXS/SANS experiments performed with the exogenous PS of animal source revealed structural changes induced by endotoxin and the ability of PxB to restore the original arrangement. Obtained results reflect accurately the situation with a native lung surfactant as confirmed by recent *in vivo* study [2] and support the idea of PxB/Cur combined therapy in neonatal medicine.

Acknowledgement: Small angle X-ray scattering (SAXS) experiments were performed at BL11-NCD beamline at Alba Synchrotron with the collaboration of Alba staff. Small angle neutron scattering (SANS) at PAXY spectrometer, Laboratoire Leon Brillouin (CEA-CNRS), CEA Saclay, France. Experiments were supported by projects APVV-17-0250, VEGA 1/0223/20, JINR project 04-4-1142-2021/2025.

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Magnetorheological properties of dense magnetic polymers

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We present results of experimental and theoretical study of effect of external magnetic field on elastic properties of dense soft magnetic polymers filled with micron-sized magnetizable (permalloy) particles. The samples were cured without magnetic field, thus with isotropic internal morphology of the particles disposition. Experiments demonstrate that under quite moderate magnetic fields the shear elastic modulus of the studied composites increased more than two orders of magnitudes. Decrease of the modulus with the valuer of the shear deformation is detected. These phenomena are explained by adhesive unification of the particles, at the stage of polymerization, into isotropic primary agglomerates.

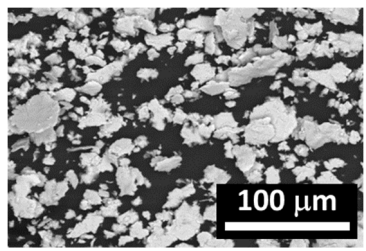

Fig.1. Image of the aggregates of the permalloy particles.

Under applied magnetic field these agglomerates are magnetized and unite into linear chains, aligned along the field. The chain length is limited by the host polymer elastic resistance to the agglomerate's displacement. Appearance of these chains significantly enforces the composite rigidity.

Some comparison of theoretical and experimental results are shown in Fig.2.

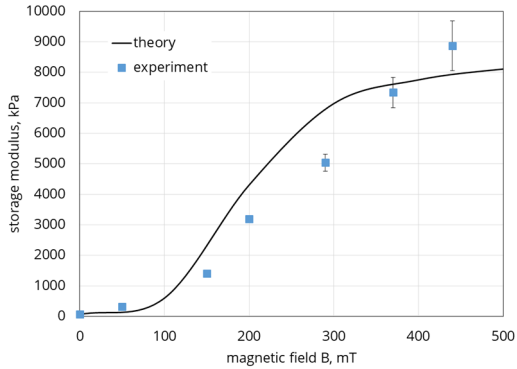

Figure2. Shear modulus vs. the applied magnetic field.. Volume concentration of the embedded particles is 30%. Modulus of the sample without the field is 10 kPa.

This comparison demonstrates that the proposed model quantitatively explains the strong magnetorheological effects in the studied dense magnetic polymers. The model also describes the decreasing dependence of the modulus on the value of the shear deformation.

ORAL

SESSION

Study of electrical characteristics of a YSZ-nanopowder chemo converter on an electreted polymer substrate

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Due to the development of innovative construction technologies in recent years, adsorption energy has become increasingly in demand. Nanoscale particles based systems that allow direct conversion of moisture adsorption energy into electrical energy are very promising [1]. Unique samples of chemo converters were obtained, in which an internal field created by an electreted polymer substrate is used to collect charge carriers localizing in the volume of the functional layer [2]. The polymer substrate was electreted at electric field 1000V/mm during 1 our at temperature 210°C with further temperature reduction to 25°C. After that, a ZrO_2+3%molY_2O_3 (400°C) nanopowder dissolved in a PVA water solution (1:10) was deposited as to the carbon electrodes as functional layer.

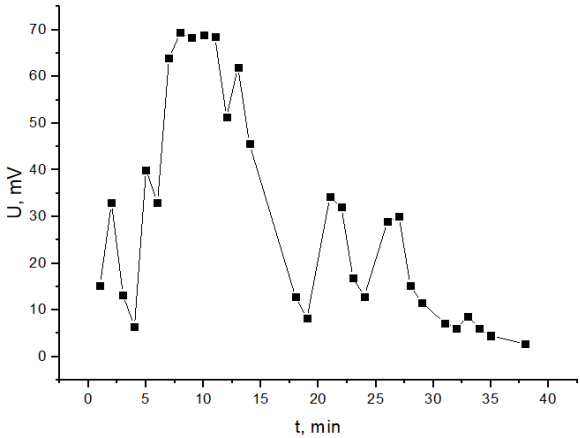

Fig. 1. The dependence of the potential difference on the electrodes on the time after placing the sample in atmosphere with a relative humidity of 99%.

The measurement of potential difference between the electrodes was made at humidity 99% on the electric load of 1 MOhm (fig. 1). It was shown that moisture adsorption lead to the increasing of the potential differences up to the 69.4 mV with a subsequent decreasing to 0 during 40 minutes.

The work performed by the cell (1,86 mkVt·s) and its average specific electric power (9,11 mkVt/m^2) were calculated. These results show the possibility of electric energy generation by this system that means that the similar nanoscale particles based systems may be used in innovative construction technologies for manufacturing of energy elements.

The study was performed in the scope of the H2020/MSCA/RISE/SSHARE number 871284 and the RO-JINR Projects within the framework of themes FLNP JINR: 04-4-1143-2021/2025 and 03-4-1128-2017/2022.

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Electrical devices based on hybrid magnetorheological suspensions: Realization, phenomenological modeling and technical characteristics

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Hybrid magnetorheological suspensions (hMRSs) are obtained by absorption of well-defined amounts of MRSs in tissues from natural and artificial polymer fibers [1, 2, 3]. Doping of natural or artificial polymer fibers with ferri-/ferromagnetic particles prevents their sedimentation and achieves ease of use in applications [4, 5].

We present the production of electrical devices (EDs), using hybrid magnetorheological suspensions (hMRSs) composed of silicone oil, carbonyl iron microparticles (20% and 40% vol. conc.) and cotton fabric. Two EDs devices are made of hMRSs, with the dimensions 30x30x2mm^3. The equivalent electrical capacity and electrical resistance of the EDs as a function of time are measured for fixed values of magnetic flux density. It is shown that the measured values are significantly influenced by the magnetic field and are stable over time. The mechanisms involved in the observed effects are described in the dipole approximation model. Together with these mechanisms, the main technical characteristics of the obtained EDs were developed and determined, namely, the nominal values of the equivalent electrical capacitance and resistance and the relative deviations from these values, the magnetocapacitive and magnetoresistive effects of the EDs. The obtained results can open research directions for the realization of magnetic field sensors, sensors, and transducers of deformations and mechanical tensions, protection equipment against electromagnetic smog, etc.

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Transversely isotropic material model of magnetoactive elastomers

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Magnetoactive elastomers (MAEs) are smart materials whose mechanical properties can be controlled by the application of an external magnetic field. They can be utilized in various engineering applications such as adaptive engine mounts, vibration absorbers, soft actuators, etc. MAEs, which typically consist of micron-sized magnetically soft particles incorporated in a non-magnetic elastomer matrix, yield a coupled magneto-mechanical response at the macroscopic scale when they are subjected to mechanical loadings in the presence of an external magnetic field. Due to the magnetic field, the induced magnetic interactions and the corresponding particle rearrangements vary the mechanical properties significantly depending on the initial particle distribution. This results in a change in the macroscopic shape of the MAE. In our earlier work [1], we studied theoretically the magneto-induced deformation, shape effect and uniaxial loadings applied to isotropic spheroidal samples along and transverse to the field direction. In this study, we investigate the magneto-mechanical response of the MAE subjected to shear deformation. The MAE yields distinct magneto-mechanical response along and transverse to the field direction, as was already found for uniaxial loadings. The modeling results firmly confirm the transversely isotropic behavior of the MAEs with a random distribution of particles. For such MAEs we propose a transversely isotropic material model as a function of the applied magnetic field and the initial shape of an MAE sample, playing a significant role in the magneto-mechanical response. We thank DFG-Research Training Group 2430 for financial support.

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Influence of magnetic field angle on the mechanical behavior of magneto-active materials

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The development of adaptable novel materials is elementary to increase efficiency of machines and reduce weight of moving parts by function integration. Concerning this field of application magnetorheological (MR) materials are a promising material class allowing the adjustment of mechanical properties by an external magnetic field. Examples for such MR materials are MR elastomers based on elastomeric materials with magnetic fillers or MR fluids based on fluids like silicon oil mixed with magnetic fillers. A key issue for operating structures with such materials in praxis is the magnetic characterization. To estimate latter the rheological properties are determined at different magnetic flux densities and for different compositions. Though in praxis different field angles are apparent a field angle dependent investigation of materials properties is not common. Known investigations for MR elastomers are limited to 0° and 90° magnetic field angles [1].

Within this work different MR materials were investigated at different field angles as well as field strength using a special shear cell called Magnetic Field Angle Testing Device (MFATD) shown in Figure 1 and introduced in [2].

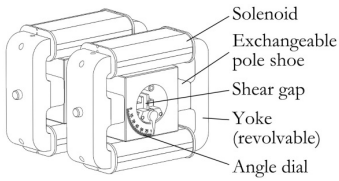

Figure 1. Developed shear cell enabling a continuous variation of the field angle

The testing device enables a continuous rotation of the magnetic field around the shear gap. To assure field homogeneity and a minimum field strength of B = 100 mT while allowing a continuous variation of field strength during testing the device uses two electromagnets. Finite element simulations were used to optimize pole shoe geometry.

First measurements were performed for Lord MRF-140CG proving general functionality of the device and showing a significant influence of the magnetic field angle

on the shear properties. Further measurements were performed for an MR elastomer with BASF CC type carbonyl iron particles in a PDMS matrix.

First experimental analysis on the field angle influence for MR elastomers and MR fluids are shown in Figure 2. As can be seen the qualitative course is clearly different for both material classes.

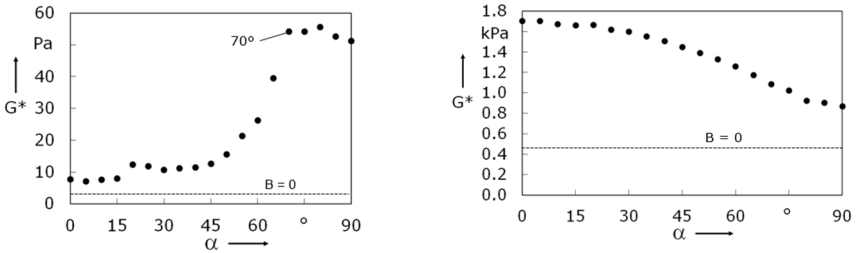

Figure 2. Complex shear moduli for different field angles at an external magnetic field strength of about 120 kA/m. left: MR fluid, right: MR elastomer.

Experimental results realized with the field angle device will presented and reasons for the different behaviors will be discussed at the conference.

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Electrostatic accelerator EG-5 in modern scientific research

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The Van de Graaff generator EG-5 is the single electrostatic accelerator at JINR. At the moment, it is capable of accelerate a beams of protons, helium ions and deuterons to energies of 2.1 MeV at a beam current of up to 100 μA. At the moment, preparations are underway for the modernization, after which the accelerator will reach its nominal parameters (4.1 MeV at a beam current of up to 200 μA).

The most suitable objects for research are smooth multilayer films. Experimental studies of the depth profiles of elements with a depth resolution of about 10 nanometers are carried out on beams of helium ions. The non-destructive techniques RBS, ERD and PIXE are used, based on beams of helium ions with energies from 1 to 3 MeV. Research is underway on multilayer high-temperature superconducting systems [1]. In addition, work is actively underway to study the processes of ion implantation of the surface of solids, the processes of structural relaxation induced by them [2,3], accompanied by oxidation [4,5] or hydrogenation [6] of the surface layers.

In terms of the development of analytical techniques, it is planned to install a microbeam spectrometer, which will make it possible to investigate not only the depth profiles of elements in the surface layer, but also to study the distribution of elements over the sample surface with a high (about 1 μm) resolution. It should be noted that in Russia there is only one operating microbeam spectrometer in Sarov.

The relatively high ion beam current (up to 100 μA) makes it possible to obtain fast monochromatic neutrons in the energy range up to 5 MeV (up to 20 MeV - after modernization) as a result of irradiation of a tritium target with deuterons (reaction D (d, n) ^{3}He). According to the Nuclear Data High Priority Request List [7], this energy range is highly demanded in modern nuclear physics research. In particular, studies of neutron-induced reactions with the emission of charged particles provide valuable information on the mechanism of nuclear reactions and the structure of the atomic nucleus, the processes of stellar nucleosynthesis, etc. It should be noted that the corresponding tasks are difficult and expensive to solve with other types of neutron installations.

At the moment, multilateral cooperation is planned with new research teams from the Russian Federation, countries of near and far abroad.

The study was performed in the scope of the Poland-JINR and the RO-JINR Projects within the framework of themes FLNP JINR: 04-4-1140-2020/2022, 04-4-1143-2021/2025 and 03-4-1128-2017/2022.

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Percolation dielectric-conductor transition in hydrated nanopowder YSZ system

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This paper shows the existence of a dielectric-conductor transition in a hydrated nanopowder system based on ZrO_2-3mol%Y_2O_3.

Wide-gap dielectric zirconium dioxide in the nanoscale state has a relatively high permittivity (ε = 25) and a high chemical activity of the surface. By changing the quantitative composition of the adsorption component, it is possible to control the energy exchange between the nanodisperse system and the external environment. The features of the transition of a hydrated nanopowder system from a non-conducting state to a state with a finite conductivity determined by the number of adsorbates are of interest for modern electronics and sensors.

Experiments were carried out with a series of obtained functional laboratory models of nanopowder sensors in the form of polymer films filled with nanoscale YSZ crystallites. Films were obtained by applying a suspension of powders in a 4% PVA solution in water to dielectric substrates with silver electrodes. ZrO_2-3mol%Y_2O_3 (YSZ) composition powders were obtained by the method of co-deposition followed by annealing at temperatures of 400°, 500°, 600°, 700°, 800°, 900° and 1000°C [1]. The distance between the electrodes is 2 mm. The dependences of the electrical resistance on the humidity were recorded at a voltage of up to 1000V on the sample. The humidity was controlled by salts in the range of 60-75%.

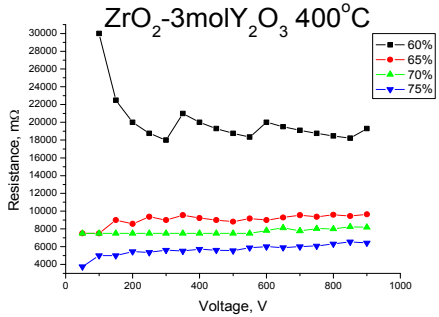

Fig. 1. The dependence of the ohmic resistance of the sample on the voltage in the element circuit.

The presence of percolation of electrical properties in the studied nanopowder systems with a particle size of 7.5 nm (annealing at 400°C) in an electric field up to 400 V/mm has been established, and it has an extreme non-monotonic character. It is also found that this feature is reduced with increasing particle size. The observed percolation jump in the electrical properties of sensors based on ZrO_2 nanopowders obtained by annealing at higher temperatures is most likely a consequence of the island nature of the distribution of hydrate shells of nanoparticles larger than 12 nm [2]. This indicates the dimensional nature of the conductivity effect of the nanopowder systems under study.

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Floating of solid magnetic and non-magnetic bodies in magnetic fluids: Inductive approach

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Field-controllable floating of solid bodies (typical size varies in the range 0.01 – 10 mm) in non-magnetic containers filled with magnetic fluids (MFs) can be used in useful technical and medical applications. This problem was studied since 1960s [1] when first MFs were synthesized. At that time almost all promising MF applications were pure technical [1, 2], thus the magnetic ponderomotive buoyancy force was studied for such special cases as levitating permanent magnets in sensors, magnetic fluid separators of non-magnetic grain materials, etc. All these problems were studied in the framework of the so called non-inductive approach, which assumes that the demagnetizing fields h generated by the container with MF are negligibly small compared to the applied field of electro- and permanent magnets $H_0 \sim 10^5 – 10^6$ A/m (MF is saturated, its magnetization $M << H_0$ and its susceptibility $\chi(H_0) \approx 0$). This approach simplifies ferrohydrodynamic problems, because the field inside MFs is assumed to be equal to H_0 and only demagnetizing fields of the solid bodies are taken into account. Nevertheless, the non-inductive approach has known limitations [2] in small and moderate fields ($H_0 \sim 10^4$ A/m) typical for biomedical applications.

The present work contains a comprehensive (experimental, numerical and theoretical) analysis of the problem in the framework of the inductive approach (MF container demagnetizing fields are taken into account). All investigation approaches are based on the common test object: a solid (magnetic or non-magnetic) sphere immersed in a cylindrical container, magnetized by a homogeneous magnetic field. The analytical and numerical results were verified by experimental measurements. All methods showed the same non-standard force behavior with two extrema for the case of non-magnetic bodies and a typical (monotonous) behavior of a magnetic body in MF (see Fig. 1). The numerical simulation was performed using Finite Element Method Magnetics (FEMM) [3]. The non-monotonic force (in case of a non-magnetic body) is explained by the competition between two mechanisms: the attraction of the non-magnetic body to the top and bottom of the narrow cylindrical container caused by the inhomogeneous demagnetizing factor of the narrow

container; and the repulsion of the non-magnetic body from the walls of the container caused by the interaction of the body's magnetic moment with its own mirror image (it was shown in theoretical analysis). The results of numerical simulations are in quantitative agreement with the experimental data, and the analytical results are in qualitative agreement with the experimental data because of the non-linear magnetization law of real MFs used in experiments.

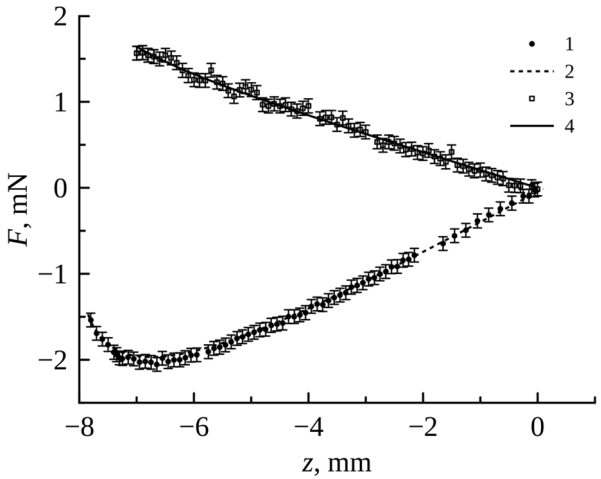

Fig. 1 Magnetic ponderomotive force F acting on the non-magnetic (curves 1, 2) and magnetic (curves 3, 4) spheres (with the radius of 3.8 mm and 4.7 mm respectively) immersed in a MF cylindrical container (radius 13.3 mm, height 23.6 mm). Vertical z-coordinate denotes the displacement of the sphere's center from the container's center. The total F(z) curve (from the bottom to the top of container) is symmetric with respect to the origin. Applied homogeneous vertical field H0 = 12.6 kA/m. Points 1, 3 – laboratory experiment; curves 2, 4 – numerical simulation in FEMM.

The work was supported by the Russian Foundation for Basic Research (project No. 20-31-70034).

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Separation of active-dipolar cubes in applied fields

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The term ”active matter” describes a class of out-of-equilibrium systems, whose ability to transform environmental energy to kinetic energy is sought after in multiple fields of science. A challenge that still remains is the creation of nanometer sized active particles, whose motion can be effectively directed by externally applied stimuli. Adding a magnetic component and therefore being able to direct the motion of active nanoparticles with an applied magnetic field proofed promising and effective in previous experimental and theoretical studies[1,2]. However, magnetic, steric and active interactions in suspension of those particles lead to unexpected properties of the systems that have yet to be discussed before developing reliable applications. In the present study, we employ molecular dynamics simulations to shed light on the internal mechanisms taking place in suspension of magneto-active nanometer sized particles in an applied constant magnetic field. We show that the orientation of the dipole compared to the active force acting on the particles determines the direction of the swimming motion while a magnetic field is applied. Particles with different orientations therefore separate under the influence of a magnetic field. However, this is only the case in dilute systems where interparticle interactions are mitigated by the low concentrations of particles. In dense systems, those interactions overpower the sorting effect and the bulk of particles perform a swimming motion in the same direction. We elucidate the underlying internal mechanisms of this effect by directing the separate components of the interparticle interactions and their influence on this behaviour.

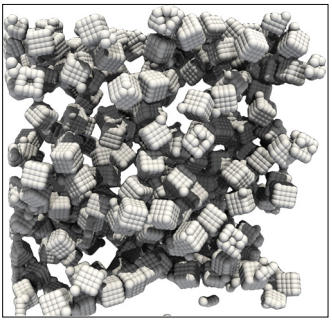

Figure 1: Snapshot of dipolar-active cube system at volume fraction **φ=0.06**

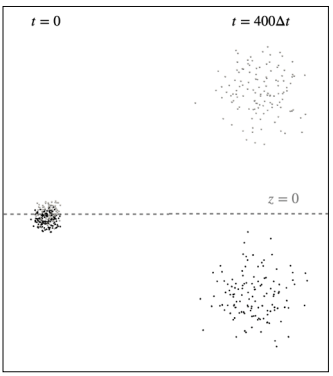

Figure 2: Separation of particles with different orientations (color coded with black and white) at low concetrations

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Neutron reflectometry for structural studies of transformer oil-based ferrofluids in electric field

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Progress in preparation of new types of magnetic fluids (MFs) based on magnetic nanoparticles (MNPs) have opened a wide range of their applications in biomedicine and technique. Electrical engineering development puts a greater demand on the cooling and insulating properties of liquid media, such as transformer oils. To enhance their performance, researchers develop various nanofluids based on transformer oils [1]. Nanofluids, formed by adding nanoscale particles to insulating oil, are stable and homogeneous suspensions that present advanced performance of electrical insulation and heat dissipation [2]. For such nanofluids, the adsorption of nanoparticles can be enhanced by applying non-homogeneous magnetic fields perpendicular to the interface [3]. Here we report self-assembling of superparamagnetic nanoparticles of classical ferrofluid under perpendicular homogeneous electric field.

Magnetite MNPs with the mean size 9 nm were synthesized by chemical co-precipitation method from aqueous solution of ferrous and ferric ions, then sterically stabilized by chemisorbing of a single oleic acid layer. Synthesis of MF was performed at IEP SAS in a well-proven way [4].

The neutron reflectometer GRAINS with a horizontal sample plane configuration installed at the pulsed IBR-2 reactor at JINR (Dubna, Russia) was employed to study the structure at the ferrofluid/solid interface under external electric fields which are close to the operating values commonly used in high voltage power engineering. The interface structure based on the obtained parameters of the adsorption layers was analyzed, which made it possible to estimate the distribution of magnetic nanoparticles in the layers. At the electrode surface in the absence of electric field we observed only wetting MNPs layer (about 16.3

nm) which was doubled and more concentrated with applying of electric field. Also it was found that application of electric field leads to formation of additional MNPs layer at the initial wetting layer with further reordering with increasing electric field more than 700 kV/m (Fig. 1). The reason of such development is polarization of the particles and their interaction as dipoles. In the static electric field, the particles are polarized and due to the high dielectric contrast between the transformer oil and magnetite, the induced dipoles are strong enough to activate the attractive interaction. Moreover the effect of electric field is visible up to 3 hours after switching the field off.

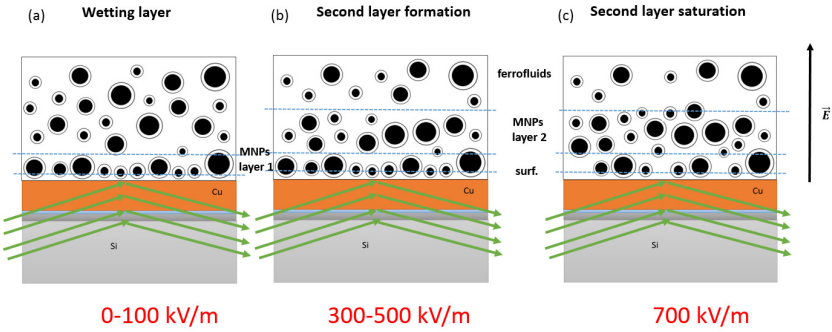

Fig. 1. Schematic drawing of NP-ordering determined from the results of neutron reflectometry: (a) wetting layer; (b) double layer on top of the wetting layer in an electric field 300-500 kV/m; (c) saturated double layer on top of the wetting layer in an electric field of 700 kV/m.

The observed self-assembled layering could be used as additional barrier at the inner surface of transformer to increase dielectric breakdown voltage of working fluids layer and advance heat transfer. As the next step for using of such materials in electric power engineering investigation of temperature effect on MF in electric field is needed.

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Complex perfluorosulfonic acid membranes with protonated nanodiamonds for hydrogen energy

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Perfluorosulfonic acid (PFSA) membranes, being copolymers with different side chain length, play an important role working in hydrogen fuel cells (FC) in portable and stationary devices with various range of power. Recent researches have confirmed the advantages of short side chain (SSC) Aquivion®-type membranes over long side chain (LSC) Nafion®-type membranes due to higher proton conductivity and better thermal stability of SSC membranes [1].

To further improve the conductive and mechanical properties of PFSA membranes we used detonation nanodiamonds (DND, particle size 4-5 nm) with positive surface potential (Z+) as nanofillers. Compositional membranes with DND content up to 3-5 wt.% were prepared by a procedure of casting the mixture of a copolymer solution with DND suspension in dimethylformamide (DMF), followed by a solvent evaporation [2].

Positive charge of DND surface made it possible to form complexes with $-SO_3^-$groups at the end of side chains of copolymer, responsible for formation of hydrophilic conducting channels in polymer matrix. We have found that a moderate amount of DND (0.5 – 1 wt.%) in SSC-DND composite is reasonable to be used as membranes with increased conductivity at higher temperatures (Fig. 1). Nanodiamond particles, having hydrophilic surface, are able to form additional centers of proton adsorption, resulting in more effective proton transfer along the DND-polymer borders. The decrease of conductivity at higher contents of DND, as well as a drop of conductivity in LSC-DND composite (Fig. 2) may indicate the closing of thin conducting channels by DND particles. Small-angle neutron scattering (SANS) experiments performed at the YuMO instrument demonstrated the remaining of ionomer peak meaning that the basic structure elements – the conducting channels – do not undergo significant changes (Fig. 3). DND particles are mostly concentrated between the bundles of conducting channels in the hydrophilic part of membranes. Thus, the optimal membranes' composition was found, and SSC material demonstrated its promising abilities to serve as membranes in FC.

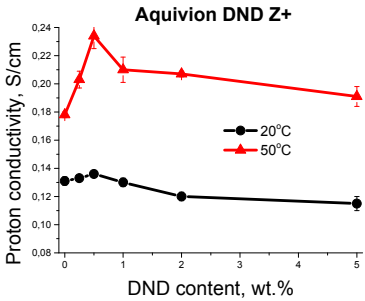

Fig.1. Proton conductivity of SSC Aquivion®-type membranes *vs.* DND Z+ content at 20 and 50°C, measured in saturated with water condition.

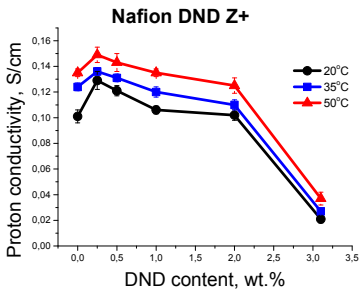

Fig.2. Proton conductivity of LSC Nafion®-type membranes *vs.* DND Z+ content at 20, 35 and 50°C, measured in saturated with water condition.

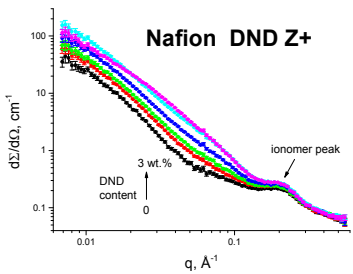

Fig.3. SANS on LSC Nafion®-type compositional membranes with DND Z+ in air-dry condition.

The work was supported by Russian Foundation for Basic Researches (gr. No 19-03-00249).

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Theoretical aspects of magnetic hyperthermia in a system of immobilized single-domain magnetic particles

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Magnetic hyperthermia is a progressive method of treatment of tumor diseases. The idea of this method is the injection of a ferroparticles into the region with the diagnosed tumor. Then the particles and, therefore, the tumor cells, are heated by an ac magnetic field. Numerous investigations show that in the temperature range ~42°C – 50°C the tumor cells die, whereas the healthy cells, being more temperature resistive, survive. Obviously, to increase the medical efficiency of this method, the accurate prediction and the control of the local temperature within the treated tissue is required.

Magnetic response of single-domain magnetic particles to an applied magnetic field is determined by two main physical mechanisms of the magnetic moment orientational relaxation. They are the Brownian rotation of particles with fixed magnetic moments and the superparamagnetic Neel rotation of the magnetic moments inside the particles due to thermal fluctuations. For ensembles of nanoparticles, suspended in some liquid carriers, known as ferrofluids, both mechanisms take place. But in the case, when particles are embedded in some polymer matrix or biological tissues, very often the particles lose their translational and orientational degrees of freedom. In this case, the superparamagnetic relaxation becomes the major mechanism determining the magnetic properties of the ensembles of such immobilized particles. In this work, we focus on the calculation of the specific loss power (SLP) of an ensemble of superparamagnetic particles with a fixed direction of the magnetization easy axes; and main attention is paid to the interparticle dipole-dipole interaction.

The monodisperse ensemble of spherical, uniformly magnetized superparamagnetic ferroparticles immobilized in a nonmagnetic matrix is considered. All particles have uniaxial magnetic anisotropy and the particle easy magnetization axes are aligned in one direction (Figure 1). External ac field **H** is oriented with some given angle to the easy axes. The rotational motion of a magnetic moment is described by the probability distribution function which is the solution of the Fokker-Planck equation. Interactions are included within the framework of modified mean-field theory [1]. Analytical and numerical

prediction is given for probability distribution function which is used for calculation of dynamic susceptibility and SLP. The dependence of SLP on direction of the field, particle concentration, intensity of the dipolar interactions, height of the magnetic crystallographic anisotropy energy barrier for internal superparamagnetic rotation of magnetic moments inside the particles is discussed.

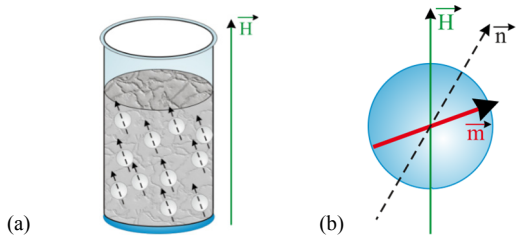

Figure 1. Sketche of the sample studied: (a) immobilized randomly distributed superparamagnetic particles with perfect alignment of the magnetic easy axes in some direction; (b) model of a superparamagnetic nanoparticle. The orientation of the particle is given by the body-fixed, magnetic easy axis vector **n**. The orientation of the particle magnetic moment **m** can be different from the easy-axis vector due to superparamagnetic fluctuations.

The study was funded by RFBR, project number 20-02-00358.

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Stabilization of magnetic fluids with poly(dimethylsiloxane) kills three birds with one stone

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More than half a century has passed since the synthesis of magnetic fluids - colloidal solutions of finely dispersed magnets. Despite the fact that the theory of magnetic fluids was built long ago and reliably [1, 2], during all this time they have not lost their relevance as an object of research. Obviously, interest in the topic of liquid magnets can be maintained by introducing into the consideration of researchers some new types of particle materials, surfactants, carrier media, etc. For example, the use of linoleic acid as a stabilizer [3] significantly expands the operating temperature range of the magnetic fluid. Stabilization of particles with polypropylene glycol [4] makes it possible to obtain magnetic fluids based on a wide range of organic media.

The recently published work [5], which describes the synthesis and properties of a magnetic fluid, in which magnetite particles were stabilized by poly(dimethylsiloxane) molecules (PDMS), is in the same theme. The use of PDMS as a stabilizer simultaneously kills not only two birds with one stone, expanding the range of operating temperatures and the variety of basic environments. (That is, it simultaneously solves the problems of works [3, 4]). It turns out that PDMS by stabilizing the particles also kills the third bird - the particles covered with a layer of poly(dimethylsiloxane) molecules do not need a carrier liquid and remain mobile without it. Thus, a new type of two-component magnetic fluids was obtained that remain operable in the absence of a basic medium. The separation of the excess of the PDMS stabilizer and magnetic particles with the PDMS coating in [5] was carried out using prolonged centrifugation. This method was chosen because of great doubts about the possibility of separating particles with PDMS shells from the excess PDMS stabilizer using coagulation [6]. However, as it turned out later, such a separation turns out to be possible. This work is devoted to the study of the coagulation stability of the PDMS of a stabilized magnetic fluid to the homologous series of saturated alcohols of normal structure and to their isomers.

It was found that normal alcohols from propanol to hexanol can be used as coagulants. Their effectiveness decreases with increasing length of the hydrocarbon chain.

Isomerization of alcohol molecules reduces their coagulation properties up to full compatibility with PDMS stabilized particles. Higher alcohols of normal structure, starting with octanol, do not mix with PDMS stabilized magnetic fluid. However, isooctanol (2ethylhexanol, the most widely used octanol isomer) is miscible in any ratio. This property can be used to develop a technology for separating isomers of higher alcohols.

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Magnetoactive elastomers based on ferromagnetic and ferroelectric particles: FORC-approach

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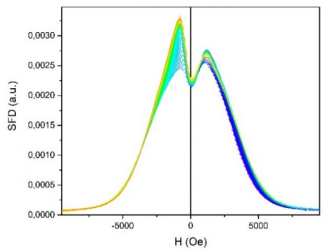
Magnetoactive elastomers – MAE – refer to composite materials that consist of polymer matrix and magnetic micro- or nanoparticles. Properties of MAE strongly depend on the type of particles and elastic modulus of polymer matric as well as particle distribution inside the matrix, namely, on the interaction between particles. Hysteresis loops of MAE usually show the process of magnetization of particles inside polymer matrix and the effect of particles spatial distribution. Meanwhile, method of FORC-analysis can provide not only consideration of magnetization process but information about local switching fields, coercivity distribution and local interaction fields [1].

We investigate the influence of ferroelectric (FE) particles, which were added together with ferromagnetic (FM) particles inside silicone matrix, on the magnetic properties of the samples. It was shown earlier that such elastomers with the mixture of FM and FE particles revealed multiferroic properties, namely, the change of magnetic properties under external electric field was found [2]. Now we would show the influence of FE particles and external electric field on the magnetization and switching properties of the composites. The influence of the composition of MAE were investigated experimentally on the following samples:

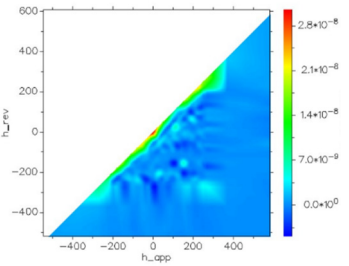
- samples with the same concentration of iron particles and different Young's modulus of polymer matrix;

- samples with the same Young's modulus and the same total concentration of iron or iron+PZT particles.

FORC-diagrams of MAE with different composition were investigated experimentally via VSM. The experimental SFD-curves of the sample with soft silicone and iron particles are presented at the Fig. 1a.



a)



b)

Fig.1. a) SFD-curves of the MAE with iron (75 mass%) particles in the matrix with 1 kPa Young's modulus, experimental results. b) FORC-diagram of the sample with FM particles with viscous-elastic and dipole-dipole interaction, simulation results.

In the frame of the model of elastic coupling between various types of particles, simulation of the magnetization curves and FORC-diagrams of the composites was carried out. To calculate particle redistribution in the system molecular dynamic approach was used. Verlet integration was used to calculate position of particles, dipole-dipole interaction between one type of particles and viscoelastic interaction (Kelvin model) between all types of particles were taken into account. In the model bulk system consists of up to 10^5 particles, moreover, the FM, FE and polymer particles were used in the sample. To avoid the problem of unsaturation of intermediate FORC-curves, the saturation state of the system was fixed. The system was smoothly brought to the new value of the return field. At that point the number of iterations was increased for additional relaxation of the system. For simulation of the presented model and visualization of the system tool was designed using C++ and Python programming languages. FORC-diagram of the sample with interacted FM particles is presented at the Fig. 1b.

In this work the theoretical and experimental FORC approaches for MAE based on different compositions were compared and analyzed.

The reported study was funded by the President of the Russian Federation Grant Number MK-716.2020.2 and Russian Science Foundation, Project No. 21-72-30032. Authors acknowledge the Russian Academic Excellence Project at the Immanuel Kant Baltic Federal University.

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Simulation of magneto-mechanical response of ferrogel samples with various polymer structure

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Ferrogels (FG) are soft magnetoactive materials, which designation comes from their composition of hydrogel matrix, filled by ferri/ferromagnetic nanoparticles. Ability to sufficient magneto-induced reorganization of internal structure and corresponding changes of topology and mechanical properties of FG samples encourages an elaboration of various applications of these materials. Especially in bio-medical tasks, such as design of micromachines (valves, pumps etc) or controlled drug delivery and release [1].

Theoretical and numerical research of FG is of importance for a developing of the materials and their applications due to complexity of direct experimental observation of FG structure on a microscale. The present work is dedicated to modelling of an equilibrium state of a small FG sample includes up to several hundreds of magnetic particles. We investigate an influence of external magnetic field and particle characteristics on material internal structure. Our model is based on coarse-grained molecular dynamics approach, which allows to choose level of abstraction optimal for a examined problem [2].

We consider FG sample with matrix possesses quasi-regular structure of network. Polymer macromolecules are simulated as a spring-bead ideal chains. Monodisperse magnetic particles have single-domain structure and uniaxial magnetic anisotropy with given energy barrier. They are placed in nodes of polymer lattice.

There is compared a behavior of FG samples with two variants of network topology: simple cubic, where each node connects 6 polymer chains, and diamond-like with 4 ‘cross-links’ per node. We examine sample magnetization, attendant forming/evolution of magnetic aggregates and changes of sample volume. Modelling shows, that material with diamond-like polymer lattice is softer and therefor demonstrates more prominent impact of magnetic forces on sample structure and topology. Moreover particle magnetic anisotropy ‘switches’ character of filed induced volume change from shrinking to swelling in samples with this variant of matrix, meanwhile for FG with simple cubic lattice only volume decrease is observed.

Calculations where performed using ESPResSo software [3] on the cluster ‘Triton’ (ICMM, Perm, Russia).

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Magneto-mechanical response of supracolloidal, magnetic, polymer-like structures

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Construction of smart materials with sophisticated magnetic response by incorporating magnetic nanoparticles (MNPs) within permanently cross-linked structures, opens up the possibility for synthesis of more complex, highly magneto-responsive systems.[1] Nanoscopic magnetic filaments (MFs) are magnetic, nano-sized colloids, crosslinked into polymer-like linear chains. They are a promising platform for engineering new magnetically controlled filtering and flow control elements in micro-fluidic devices. Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, finally opened the door towards synthesis of MFs with desirable mechanical properties.[2,3,4] Using programable DNA origami assembly, we created scaffolds that can serve as blueprints for chain-like assembly of MNPs (i.e. 20nm, streptavidin coated magnetite NPs), allowing them to assemble in to structures possible only for anisotropic and selective interactions. Using MD simulations we have studied how possible crosslinking scenarios and magnetic nature of monomers (ferromagnetic or super-paramagnetic) influence equilibrium properties of MFs.[5] Filaments with super-paramagnetic monomers have proven to maintain a desirable magnetic response in various crosslinking approaches, making them a more flexible choice. In strong applied fields, MFs with super-paramagnetic MNPs have similar magnetic properties to ferromagnetic ones, while exhibiting higher susceptibility in low fields. Furthermore, they exhibit an interesting tendency to bend their backbone locally, rather than to fully stretch along the field. In this contribution, we elucidate an interesting phenomenology of MFs, by examining their behaviour in a Langevin thermostat (equilibrium properties) and explicit solvent representations using the Lattice Boltzmann method (dynamics in rotating magnetic fields). Magnetization of super-paramagnetic monomers is taken into account in an accurate manner, inclusive of non-linear contributions.

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Theoretical modeling of circulation flows in a magnetic fluid

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The main problem in the treatment of stroke is associated with the fact that thrombolytic drugs diffuse very slowly in thrombosed vessels. The American company Pulse Therapeutics has found a solution to this problem, in which magnetic micro- or nano-sized particles are set in rotational motion using an alternating magnetic field, capable of generating circulation flows in thrombosed vessels [1]. These currents greatly enhance the convective transport of the drug to the blood clots in the vessels. There is still no physical understanding of the origin of oscillatory flows, which are created by moving and rotating magnetic particles. In this work, a theoretical model is proposed that takes into account the motion of ferroparticles and induced fluid flows inside the channel under the influence of alternating inhomogeneous magnetic fields. The obtained amplitudes of the fluid velocity are compared with the values required for efficient drug delivery to blood clots in real situations.

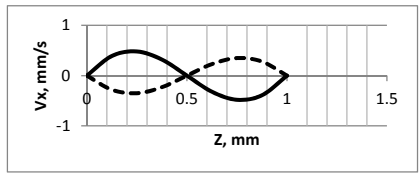

Figure 1 - The longitudinal component of the velocity v_x with respect to the z coordinate at a fixed x = 10 mm. Dotted line: time t = 0.5 s; solid: t = 1 s. The angular frequency of the field is $\omega \sim 10$ rad/s; volume concentration of particles in the center of the cloud $\Phi_0 = 0.01$; gap thickness l = 1 mm.

The results obtained show that a rotating magnetic field with an amplitude of about 17 kA / m and a frequency of about 10 rad/s in a channel 1 mm wide can induce a circulation flow with a velocity amplitude of about 0.5 mm / s (see Fig. 1), which may be of interest from the point of view of targeted drug delivery in blood vessels.

The work was carried out with the financial support of the Russian Foundation for Basic Research, projects 18-08-00178, 19-31-90003, 19-52-45001, 20-02-00022.

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Magnetic nanogels in a constant magnetic field

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Nanogels (NGs) with multifunctional magnetic nanoparticles (MNPs) have shown the ability to selectively destroy cancer cells in vivo without causing visible damage to healthy organs [1]. The inclusion of MNPs within NGs also provides an additional method for controlling their properties by means of an applied magnetic field.

Our analysis of the suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel and self-assembly in the given system are highly affected by the strength of the dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here we study a suspension of magnetic NGs in a constant external magnetic field *in silico* using the molecular dynamics method [3]. Each NG is initially modeled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. Locations of MNPs inside the gels are random as well.

We find that even small fields contribute to substantial changes in the arrangement of both embedded MNPs and NGs as a whole. But what is much more curious is that the polymer matrix of nanogels strengthens the magnetisation of free MNPs.

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Influence of ion energy and mass on the TiO_2/SiO_2 transition layers

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Influence of energy and mass of the implanted ion on the mixing process of TiO_2/SiO_2 interfaces were investigated using RBS method. The specimens were irradiated with the noble gas ions Ne^+, Ar^+, Kr^+, Xe^+ at different energies of 100, 150, 200, 250 keV. The irradiation was carried out at the room temperature with the fixed value of the ion fluence at 3×10^{16} [ions/cm^2]. The RBS method was used for determining the elemental depth profiles of the samples. The 1.5-MeV He^+ ion beam was directed to the samples under the incident angle 60^0 towards the normal of the sample surface. The RBS spectra were collected at a scattering angle of 170^0 away from the beam incident direction. The primary parameters that were measured by the experimental technique are used to characterize the mixing process. Shifting of the Ti, Si energy edges from RBS spectra indicated to the mixing of the atoms across the interface of TiO_2/SiO_2 systems that lead to forming of the transition area between the layers. Mixing amount was quantified by changing thickness of transition layers well as the TiO_2 layers which was correspond to variation FWHM of the Ti peaks. We have found that the relative thickness of transition layers increases linearly with increasing of energy, contribution of decreasing FWHM to mixing is not significant. The displacement of the Ti atoms across the interface is predominant contributing to the broadening of the mixed layers towards the substrate more than that in the opposite direction. The influence of ion mass on changes in the thickness of the transition layers, however, is not described by a linear relation. Mixing rate strongly depends on the heavy ions, it is about 2.8 and 7.6 times larger for Kr and Xe than that of Ne. The Monte Carlo

simulation was performed using SRIM code for understanding as well as for explanation of these effects based on the depth-dependent damages and the defect concentration profiles.

The study was performed in the scope of the Poland- JINR and RO-JINR Projects within the framework of themes FLNP JINR 03-4-1128-2017/2022.

Cr(VI) adsorption on ordered mesoporous silica functionalized with aminopropyl groups by co-condensation and post grafting

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Morphology and adsorption properties of mesoporous silica functionalized with APTES by the co-condensation and the post grafting methods were evaluated. Nitrogen sorption, small angle neutron and X-ray scattering (SANS and SAXS) demonstrated high surface area and well-ordered hexagonal pore structure suitable for applications as adsorbents of metals from waste waters. SAXS and SANS data show that the increase of the amount of organic silica precursor in the co-condensation process leads to the decrease of the long-range order of the parallel channels. The co-condensation of tetraethoxysilane (TEOS) and 3-aminopropyl triethoxysilane (APTES) resulted in higher metal sorption capacity of the materials compared to post-synthesis grafting of aminopropyl groups onto the mesoporous silica particles. From the performed studies it was found that adsorption capacity of Cr(VI) was almost ten times higher for the material prepared by co-condensation compared to the one prepared by post-grafting (q_{exp} = 85.5mg/g vs. q_{exp} = 9.4mg/g).

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Ferromagnetic nematic phases of charged magnetic nanoplatelets

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In recent decades, advances in synthesis techniques have opened up a new subfield in the study of magnetic soft matter: the study of anisotropic and anisometric magnetic colloidal suspensions. The persistent interest in investigating and refining anisotropic colloidal systems comes from the knowledge that colloidal anisometry can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter[1]. For instance, a suspension of discotic mesogens with a dipole moment perpendicular to the long axis of the particle can form a macroscopic ferromagnetic nematic phase at room temperature[2]. While the phase behavior of hard platelets is already well-known, the influence of the added dipole moments on the isotropic to nematic phase transition is not yet fully understood. This contribution will focus on the computational work to characterise the phase behavior of such systems, recreating them through Molecular Dynamics simulations in different approximations (raspberry and Gay-Berne), then studying the influence of parameters such as the dipole moment or aspect ratio on the phase transition, as well as analysing the structural properties of the system in different phases.

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Coarse-grained model of a magnetic microgel

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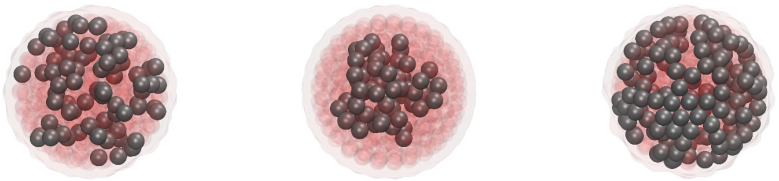
Magnetic microgels are hybrid soft hydrogel entities (up to several hundred nanometers), within which embedded iron oxide magnetic nanoparticles (MNPs) [1,2] are distributed. The cross-linked mesh structure of the hydrogel provides a sponge container capable of transporting liquid substances (e.g., dissolved drugs) whereas the MNP subsystem makes a magnetosensitive 'drive' that enables one to move the microgel remotely and controllably and, if necessary, release its cargo as the destination is attained.

The applicationally relevant functional features of microgels come out as a result of the interplay between elastic properties and topology of the supramolecular polymeric structure, magnetic specifics of the MNPs, and the manner in which the magnetosensitive elements are distributed over the gel volume. The theory and numeric modelling of the microferrogels are yet at their beginning and this is one of the most challenging points of the magnetic soft matter science. In this work we present a flexible and tunable computer tool developed for simulating a single microgel entity with the aid of a well-tested approach – coarse-grained molecular dynamics [3,4] implemented in the framework of ESPResSo platform [5].

As a starting point of the model, the microgel is configured as a dense clot of beads (coarse grains) of identical size. Two types of the beads are introduced: they are either MNPs or polymeric globules. By connecting the beads by elastic bonds (springs) a wide variety of structures might be arranged in accordance with a beforehand-chosen plan; for example, the number of nearest neighbors and the number and rigidity of the bonds between them are easily customized. The magnetic properties of MNPs are defined by the direction and magnitude of their dipolar moments. The assembled bead-spring construction with a given size and pre-determined volume fractions of both components is placed in a thermostat under constant temperature conditions under zero magnetic field. The coarse-grained calculation process is started, and the system is subjected to it until it equilibrates. Repeating the procedure several times, one obtains a number of replicas of the same sample. The ground state (zero external field) of a microgel is analyzed for different degrees of crosslinking and initial types of spatial distribution of MNPs (see Figure 1): 1) randomly

filled microgel, 2) “magnetic core – polymeric shell” microgel and 3) “polymeric core – magnetic shell” microgel.



a) b) c)

Figure 1. Initial MNPs distributions in microgel sample:
a) randomly filled, b) magnetic core – polymeric shell, c) polymeric core – magnetic shell.

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The ensemble of immobilized superparamagnetic dipoles: The role of the particles' distribution in the sample

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The design of magnetic soft materials has steadily progressed: it is now possible to embed magnetic particles into polymer matrices. Improving the synthesis technology and developing methods for using magnetoresponsive elastomers and ferrogels requires solving fundamental problems related to predicting the behavior of ensembles of magnetic particles in a polymer matrix. A different distribution of magnetic nanoparticles inside the sample leads to a significant change in its bulk properties [1,2].

To study the effect of dipole-dipole interparticle interactions on the static thermodynamic and magnetic properties of an ensemble of immobilized superparamagnetic particles, two types of the particles' distributions at the sample volume were considered: (i) on the nodes of the regular cubic lattice and (ii) by the random way. The response of the particles to the external magnetic field occurs by the Neel mechanism due to their magnetic moment rotation inside the nanoparticle [3]. It was assumed that the directions of the easy axes for all particles were parallel to each other and directed at an angle to the external magnetic field **H**: it was described using the polar and azimuthal angles φ and θ, respectively. The model of polymer is illustrated on the Figure 1.

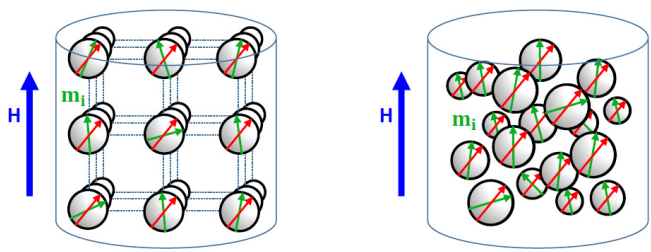

Figure 1. Monodisperse system of immobilized single-domain superparamagnetic dipoles at external magnetic field **H**. Container has the cylinder form strongly elongated along **H**. Particles' distribution at the volume can be (a) at the nodes of a simple cubic lattice or (b) by the random way.

The described model was studied using both theory and computer simulation, taking microscopic discrete structure explicitly into account. Theoretical approach is based on the expanding of the Helmholtz free energy into a classical virial series up to the second virial coefficient. In addition to the pair interparticle dipole-dipole interactions, there was taking into account the interactions of magnetic moments with the easy axes and the external magnetic field. It was found that in a zero magnetic field the contribution of the dipole-dipole interparticle interaction to the Helmholtz free energy ΔF for the first system (Figure 1 a) depends on the polar angle φ, while for a random distribution of ferroparticles in the volume (Figure 1 b) there is no such dependence.

The analytical expressions of the Helmholtz free energy for both textures allow to obtain theoretical predictions for the static magnetization and the isochoric heat capacity as functions of the height of the magnetic crystallographic anisotropy energy barrier for the internal superparamagnetic rotation of magnetic moments inside the nanoparticles, measured by parameter σ, and the intensity of the dipole-dipole interparticle interactions measured by λ. These characteristics turned out in a good agreement with the Monte-Carlo simulation data in the region of low and moderate values of σ and λ. In zero and moderate external magnetic field, the new theory allows to describe the numerical calculations much more efficient than the ideal approximations [3], for which the interparticle dipole-dipole interactions where neglected.

The obtained results for the thermodynamic and magnetic properties of the immobilized superparamagnetic nanoparticles can be important in the development of functional magnetic materials with controlled properties.

The study was funded by RFBR, project number 20-02-00358.

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Isoscattering point in SANS contrast variation studies of magnetic fluids

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Small-angle neutron scattering (SANS) is widely used in structural diagnostics of magnetic fluids [1,2]. Carrying out hydrogen/deuterium isotopic substitution in liquid media of magnetic fluids makes it possible to adjust the neutron scattering length density of the solvents, ρ_{solv}. This is the basis of the SANS contrast variation technique [3].

There are specific points at which the neutron scattering intensity of liquid nanosystem is independent of the scattering length density contrast between dispersed particles and solvent. These points, q^*, are referred to as 'isoscattering points' [4]. q^* is inversely proportional to the particle size. Usually, the nature of the isoscattering point is associated with the high symmetry of the nanoparticle shape and low polydispersity. However, it has been observed in the SANS data of various magnetic fluids [5-7], despite the fact that they are characterized by a polydispersity of 25-40%. An example of such SANS contrast variation experiment on an aqueous magnetic fluid is shown in Figure 1.

To explain this phenomenon, it seems promising to use the method of basic functions [3], namely the expansion of the scattering intensity in a series in contrast, $(\rho_{part} - \rho_{solv})$, where the basic functions $I_s(q)$, $I_{cs}(q)$ and $I_c(q)$ are the coefficients. Within the framework of this formalism, the condition for a isoscattering point is relation $I_s(q^*) >> I_{cs}(q^*)$, $I_c(q^*)$.

This communication discusses the conditions for observing an isoscattering point for polydisperse core-shell structures as a model of magnetic fluids with steric stabilization, as well as additional possibilities of structural characterization via SANS based on this effect.

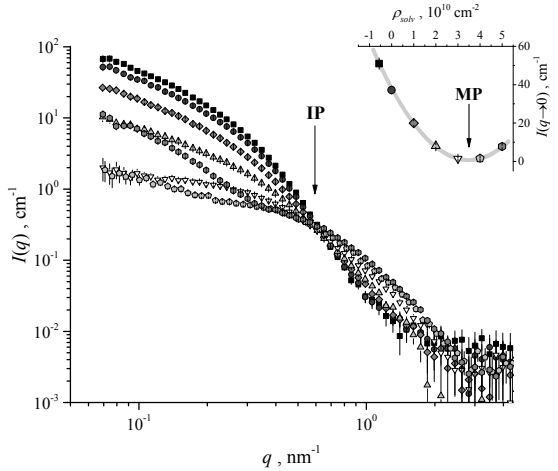

Figure 1. Changes in experimental SANS curves with contrast variation for Fe_3O_4–2·DBSA–H_2O magnetic fluid. Curves are plotted with the same color and point style as the corresponding points in inset, where the change in the forward scattering intensities with varying solvent SLD is shown. Arrows indicate isoscattering point (IP) as well as effective match point (MP) corresponding to the minimum of quadratic dependency (solid line).

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Development of modified filler for soft magnetic composite materials

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Soft magnetic materials are of great interest due to their property to switch magnetic polarization under the influence of small magnetic field. The process of switching has been found an application in different scientific and industrial areas. There are transformers, sensors and protection from electromagnetic interference.

It's well known that the most materials with these properties are alloys with different chemical compounds. Because of increased demand for polymer materials it's necessary to develop special fillers for getting soft magnetic properties.

In our work the modified carbon fiber (CF) with magnetite particles was considered as the filler for soft magnetic composites. This choice was connected with small specific weight and good physical mechanical properties of CF.

Modification of CF was carried out in magnetic fluid using ultrasonic treatment on a Sonopuls HD 3200 (Bandelin, Germany) for 1 hour. Then the filler was washed by distilled water and dried at 100 °C for 24 hours. The modification was performed 3 times.

An analysis of the surface structure of the modified fibers was carried out using a FEI Quanta 650FEG scanning electron microscope (FEI, USA) (Fig.1).

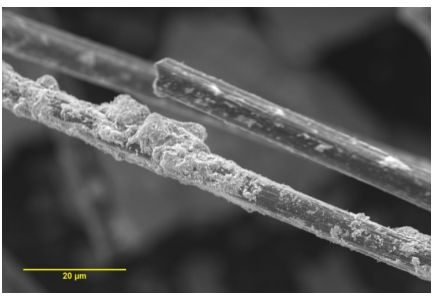

Fig. 1. SEM-image of modified CF by magnetite particles

The TGA method was used to make a preliminary estimate of the amount of deposited magnetite on the surface of carbon fibers, which was 17, 23 and 34 % for stages 1, 2 and 3, respectively.

By the Raman spectroscopy (SENTERRA (Bruker, Germany)) it was found that the coating on the CF is magnetite. For all Raman spectra, a peak 664 cm^{-1} corresponding to magnetite is usually observed and represents a symmetrical section of oxygen atoms along Fe-O bonds corresponding to the A1g mode. The peaks at 369 and 504 cm^{-1} correspond to the peaks of partial oxidation of magnetite to maghemite (γ-Fe_2O_3). Two characteristic bands of D (defects) at 1343–1356 cm^{-1} and G (graphite) at 1586– 1594 cm^{-1} are usually observed and connected with degree of graphitization of CF.

To study the magnetic properties, model samples of polymer materials based on ED-20 epoxy resin were made. The filling was 1, 3 ,6%wt.

The magnetic hysteresis curves m(H) for Jc calculation at different temperatures as 10 and 28 K were determined with a commercial Vibrating Sample Magnetometer, VSM-9T (Cryogenic). It is observed that all the hysteresis loops are very narrow with small coercive magnetic fields.

The reported study was funded by RFBR and Perm Territory as part of a scientific project no. 19-43- 590024 p_a. The work was carried out using the equipment of The Core Facilities Center «Research of materials and matter» at the PFRC UB RAS.

POSTER

SESSION

Thermoplastic polyurethane: Phase mixing and phase separation upon accelerated aging

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We studied the microstructure changes occurring in a commercial polyester polyurethane, compression molded Estane 5703 films exposed to accelerated aging treatment with elevated temperature and humidity, and irradiation by high energy gamma rays with a dose up to 500 kGy. The structure has been studied by small-angle X-ray and neutron scattering (SAXS and SANS), Fourier transform infrared spectroscopy (FTIR), gel permeation chromatography (GPC), differential scanning calorimetry (DSC) and X-ray diffraction (XRD).

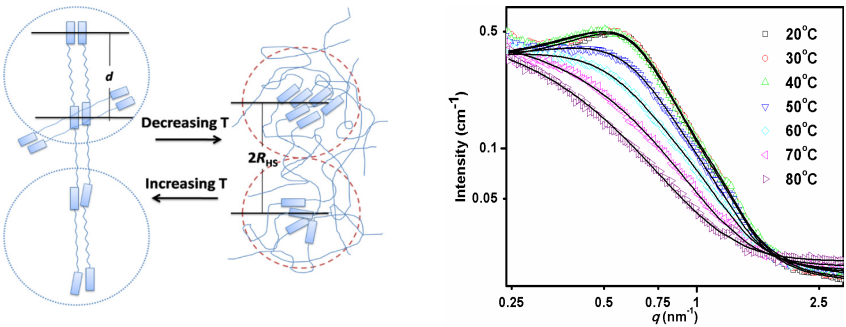

Figure 1. Structural changes with temperature: mesophase mixing upon temperature increase, and phase separation on cooling. SAXS data.

During heating, above 40 °C, the scattering show the mixing of hard domains (MDI-BDO) with soft matrix (PBA), with a sharp increase of the hard domain distance at 50–60 °C. Between 60 and 90 °C, a newly-observed ordering appeared as the formation of a distinct mesophase with a repeat distance of 5.15 nm. After cooling, the domain structure partly recovered, but did not reach the original state after 3 month storage.

In the accelerated aging experiments, GPC data showed a progressive shortening of polyurethane chains with aging in humid conditions, and FTIR showed an increase of the number of inter-urethane H-bonds.

The small-angle scattering shows that the interdomain distance and domain size increase with a higher humidity and longer aging time. Conversely, in the irradiated films, the hard domain size decrease: FTIR shows that the cross-linking occurred among the secondary alkyl radicals, and the interactions in the hard domains weakened because of the loss of inter-urethane H-bonds. GPS data also indicate the formation of a fraction of interconnected polymer chains.

In summary, the accumulated data reveal that the reduced steric hindrance caused by hydrolysis of ester links in polybutylene adipate residues promotes the organization of hard segments into domains, leading to the increase of domain size and distance, as well as phase segregation. The samples irradiated in water exhibited a stronger aging effect than those irradiated in air.

These findings provide insight into the effects of various treatment conditions on the microstructure of aged polyester urethane from the molecular to nanoscale level.

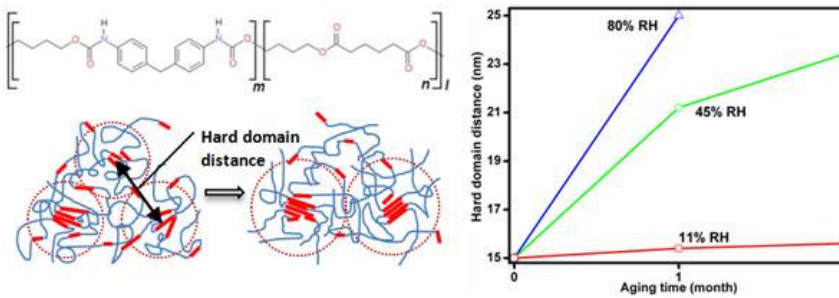

Figure 2. Chain scission and domain reorganization during accelerated aging in humid conditions.

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Numerical modeling of the dynamic susceptibility of an ensemble of immobilized magnetic particles with aligned easy magnetization axes

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Magnetic nanoparticles already proved their applicability in different areas. Embedding a large number of magnetic nanoparticles into a liquid or polymer matrix makes it possible to control the properties of a composite material using an external magnetic field. Such materials, so-called magnetic soft matters, include ferrofluids, magnetic elastomers, ferrogels, and various biocompatible magnetic filling. In the last decade, a new wave of interest to magnetic soft matter appears due to their connection with using such material in diagnostics and therapy.

In this work the dynamic magnetic response of immobilized superparamagnetic nanoparticles to an ac field with an arbitrary amplitude is studied using numerical simulations. The nanoparticles are considered to be distributed randomly within an implicit solid matrix, but the easy axes of the particles are aligned parallel or perpendicular to the ac magnetic field. Modeling of dynamic response is based on the Fokker-Planck-Brown equation in which the interparticle dipole-dipole interactions are included within the framework of the modified mean-field theory [1]. The numerical solution of Fokker-Planck-Brown equation is based on an unconditionally stable scheme for convection-diffusion problems [2]. The effects of the magnetic crystallographic anisotropy barrier, the ac field amplitude, and the interparticle interactions on the dynamic magnetization, susceptibility, and relaxation time are analyzed. The numerical results are compared against a theory [3] reliable in a weak ac field, and the excellent agreement is obtained.

The study was funded by RFBR, project number 20-32-90209.

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On the $CoFe_2O_4$/LA/SDS-Na/H_2O ferrofluid structure. Effect of dilution and temperature

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Studies of samples of ferrofluid $CoFe_2O_4$ / LA / SDS-Na / H_2O with different concentrations were carried out using the method of small-angle neutron scattering (SANS). The ferrofluid was prepared at the Institute of Technical Chemistry, Perm [1, 2], with $CoFe_2O_4$ nanoparticles obtained by co-precipitation of $Fe(OH)_3$ and $Co(OH)_2$ and stabilized by adsorption of lauric acid (LA) on ferrite particles, followed by peptization of the hydrophobic precipitate in an aqueous solution of sodium n-dodecyl sulfate (SDS).

The experimental data were processed using the SASView program. For the best fit in the Q region, $0.006 \le Q \le 0.07$, was chosen the following functional form [3]:

$$I(Q) = \begin{cases} \frac{G}{Q^s} \exp\left[\frac{-Q^2 R_g^2}{3-s}\right] Q \le Q_1 \\ \frac{D}{Q^m} Q \ge Q_1 \end{cases} \quad (3)$$

The first branch in the definition (3) represents the generalized Guinier law, where s is a nondimensional parameter that characterizes the shape of the scattering objects (for sphere, for rods, for plates), and are used as scale constant and

$$Q_1 = \frac{1}{R_g}\sqrt{(m-s)(3-s)/2}. \quad (4)$$

The second branch describes a power law dependence characteristic to the self-affine structure in the form of mass fractals or of surface fractals. In the case of mass fractal, the

fractal dimension varies between 2 and 3 and is equivalent to the Porod exponent. For the surface fractals the fractal dimension is higher than 3 [4, 5].

The analysis of the SANS curves and the modelling of concentration effects on the CoFe2O4 / LA / SDS-Na / H2O ferrofluid system are carried out. The structural effect of temperature change from t = 22 ° C to t = 43 ° C and return to 22 ° C is also analysed.

When modelling the experimental curves, the approximation of a spherical particle is considered. The radii of gyration are determined for each situation. The radius of gyration values increases with decreasing particle concentration, while the Porod exponents change in the opposite way. It increases with increasing concentration of particles in a particular non-linear dependence. An increase in the Porod exponents was noted with the increase in the concentration of particles for each temperature.

Higher values for radii of gyration as well as for the Porod exponents, for the high temperature, can be explained as a consequence of the aggregation of some of the particles as an effect of the dilution. In each case, the Porod coefficient gives a measure of the fractal properties characteristic for specific particle agglomeration behaviour [6].

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Effect of the proteoliposome structure on the photocurrent during their sorption on the lipid membrane

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One of the common ways of using model membranes is to study the functional features of light-activated ion channels and pumps. In this work, the adsorption of proteoliposomes (PLs) on planar bilayer lipid membranes (BLM) approach was considered [1]. These liposomes must be small enough. Size indirectly ensures that the protein is in its native orientation and that the liposomes are unilamellar. However, the structure and size of liposomes depends on many parameters: pH, the presence of metal ions (especially bivalent), the method of production, storage time and some other. The use of non-unilamellar liposomes can lead to changes in characteristic photocurrents, which is described in this work.

The installation used in this work is a container made of a dielectric material with a hydrophobic surface. The container consists of two compartments separated by a wall, in which there is a small hole tapering towards the center. During the experiment, the container filled with a buffer so that the hole is below the liquid level. Then a lipid membrane is installed on the hole. During incubation, it becomes thinner, becoming a lipid bilayer, which is characterized by optical changes. Further, on one side of the membrane, liposomes are added, the lipids in which are charged with the opposite to the membrane sign. During incubation, liposomes reach their maximum sorption on the membrane. Using electrodes located on opposite sides of the membrane, the operator measures the electrical parameters of the received object.

In this configuration, the hole is illuminated with a 1 W white light bulb and a response signal is observed. The standard answer is shown in Figure 1. Light is on at 0 sec and off after 10 sec. The peak corresponding to the light on and the proton pump activation takes less than 0.5 seconds. This is followed by a constant current. After turning off the light, the current also quickly returns to the value before light on. When an external voltage is applied in the range from -70 mV to +70 mV, the answer does not change significantly. Then 10

mM carbonyl cyanide m-chlorophenyl hydrazone (CCCP) was added. After 10 minutes the measurements were repeated (Figure 2). The sign of the photocurrent change relative to the baseline before illumination became the opposite. Time of the transition to a constant value after the transient current is more than 10 seconds. When single-layer liposomes are used, the characteristic changes after the transient current do not change significantly after the addition of the protonophore.

These liposomes were examined by dynamic light scattering (DLS). It was found that the diameter of the liposomes used was 128 ±15 nm.

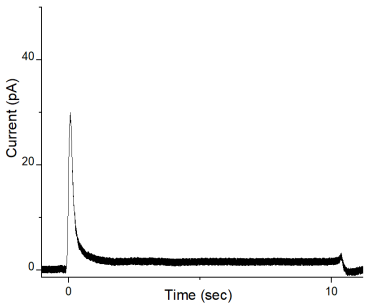

Figure 1. Change in photocurrent under illumination of liposomes with a proton pump, when an external voltage of 50 mV is applied

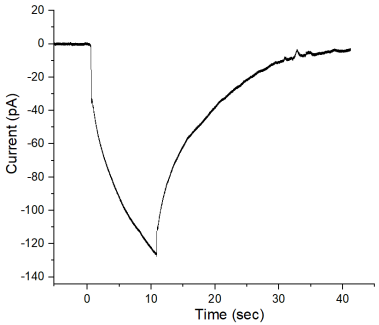

Figure 2. Change in photocurrent under illumination of liposomes with a proton pump, after adding CCCP, and external voltage 60 mV

Thus, it is assumed that this effect is due to the fact that the liposomes used in the experiment are different from the unilamellar ones.

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Study of the systems with magnetic nanoparticles by muon spin rotation (muSR) technique

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We used polarized positive muons (μSR[1]) to study the magnetic properties of the ferrofluids.

The paper presents an experimental study of the ferrofluids based on magnetic nanoparticles of Fe_3O_4[2] and $CoFe_2O_4$[3] dispersed in water with a different nanoparticles concentration. In this study, it was determined that the structure and magnitude of the magnetization of a ferrofluid depends on the viscosity of the liquid itself.

We studied the difference between the magnetic properties of ferroliquids at the cooling at FC and ZFC conditions. Figures 1 and 2 presents the example of obtained data.

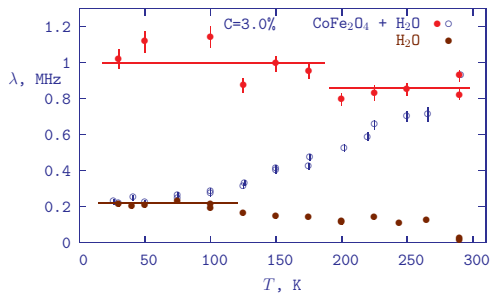

Fig.1 The temperature dependencies of the relaxation rate of the muon spin precessions at ZFC (open circles) and FC (closed points) conditions at 500 G.

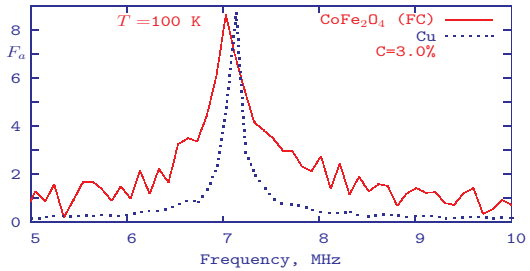

Fig. 2 The Fourier spectra of the μSR data for Cu and for sample with concentration of the cobalt ferrite nanoparticles of 3% at FC conditions of the cooling .

We analyzed data from the point of view of studying the properties of an ensemble of single-domain magnetic nanoparticles.

It is shown that at room temperature (290 K) and an external magnetic field of 527 G, the observed additional magnetization. In a small fraction of the sample under study (~ 20%), negative magnetization (diamagnetism) is observed. At low temperatures (~ 30 K), the samples behave like a paramagnet in a magnetic field. For the first time experimentally using the μSR method, the magnetic field inside and in the immediate vicinity of the $CoFe_2O_4$ nanoparticles was measured, thus a direct measurement of the magnetization of a nanoscale object was made.

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Effect of concentration and ionic strength on the structure of linear poly(N-isopropylacrylamide) thermoresponsive polymer

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In the past few decades the importance of polymers rapidly increased due to their potential usage in nanotechnology. The stimuli responsive polymers are in the hot spot of polymer science since their structure can be tuned by changing the physical chemical properties of the environment [1]. The most extensively studied member of this class of materials is the poly(N-isopropylacrylamide) thermoresponsive polymer (PNIPAAM). PNIPAAM has a lower critical solution temperature (LCST) at around 32 °C [2][3]. The LCST can be changed by copolymerization of more hydrophobic or hydrophilic comonomers [2][3][4][5], and with the change of the solution environment, e.g., low molecular weight inert electrolytes in the aqueous phase [5]. Below the LCST, the pNIPAAM chains are soluble in water, however, above the LCST, phase separation takes place. There are several studies dealing with the self-assembled nanostructures induced by the phase transitions of pNIPAAM above the LCST (e.g., in the case of PEG-b-pNIPAAM block copolymers) [6]. Most of the published work has focused on the micelles formed at temperatures above the LCST, where the collapsed pNIPAAM chains form the core and the hydrated PEG chains form the shell [7]. In our recent study we showed the structural changes of coecarvates formed by oppositely charged block copolelectrolytes bearing with PNIPAAM blocks in the function of temperature and solution ionic strength [8].

Despite the variety of applications of pNIPAAM in polymer technology the concentration dependence of the phase transition has not been investigated. In our work we used small-angle X-ray scattering to monitor the concentration dependence of the effect of ionic strength and temperature on the LCST. pNIPAAM with 100 000 Da molecular mass was used. Three different concentration (1 wt%, 2.5 wt% and 5 wt%) were investigated in pure water and 50 mM NaCl, as a function of the temperature.

In order to obtain detailed structural information of the polymer, Debye chain form factor was fitted to the experimental scattering curve below the LCST. The high

concentration of polymer causes a concentration effect due to the interaction of the chains. These effects were described by the random-phase approximation [8] structure factor. The obtained structural parameters are shown in Fig.1.

Our results showed that by increasing the concentration of the PNIPAAM shifts the LCST to a lower temperature. We also revealed that the polymer is in a more extended form (radius of gyration in Fig.1) in the presence of indifferent electrolyte and the attractive force between the segments (second virial coefficient in Fig.1) increases between the polymer segments.

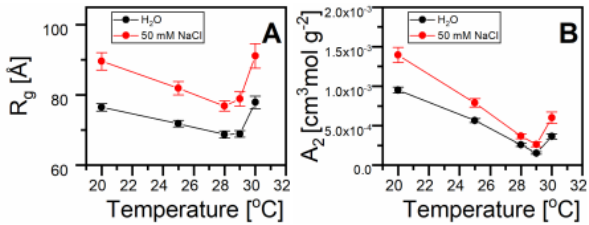

Fig.1. Fit results from SAXS data: (A) root-mean-square radius of gyration and (B) second virial coefficient as a function of temperature.

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Nanocomposite alginate hydrogels for 3D printing applications

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Alginate is a natural polysaccharide extracted from brown algae. It is linear structure consists of alternating β-D-mannuric (M) and α-L-guluronic (G) acid monomers. Sodium alginate hydrogels can be easy prepared by crosslinking with 2x valence metal cations. The bond between the alginate polymer chain and divalent cations is usually described using the "eggs box" model. Due to biocompatibility and ease way of gelation, alginate hydrogels have been used in various areas of industry, such as cosmetology, biomedicine, engineering et al. Recently they began to be used as bioprinting inks for a tissue engineering [1].

For 3D-bioprinting, calcium chloride is mainly used as a crosslinker for alginate. The polymer forms a gel with dynamic crosslinks. The crosslinks break when stress is applied to the gel after which, and in the absence of stress, the chains can merge again and gel structure recovered. This is a thixotropic property of the alginate hydrogels. This feature of alginate hydrogels important for 3D printing, since the ink after extrusion from the printer nozzle must recover elastic properties and keep its shape. However, mechanical properties of alginate do not allow obtaining the required resolution for printing; therefore, the search for the properties of biocompatible fillers to increase the mechanical properties without loss of thixotropy is urgent now. As such additives, we offer halloysite natural clay nanotubes, which possess biocompatibility and cytocompatibility. Halloysite has been used as nanofiller for polymer nanocomposites [2], but has not been studied as extender for alginate hydrogels.

The studies were carried out with sodium alginate hydrogels modified with aluminosilicate nanotubes in the range below and above the overlap concentration of the tubes. All gels prepared at pH = 7.2±0.1. Mechanical properties have been studied using rheology. The structure was investigated using the SAXS.

The research obtained nonlinear effects of halloysite on the elastic modulus, linear viscoelastic response, yield stress and recovery rate of the alginate hydrogels. The latter were prepared with different amount of polymer chains and degree of cross-linking. The nanocomposite hydrogels possess shear thinning behavior and recover initial structure and properties after injection at the presence halloysite nanotubes even above overlap

concentration. The developed nanocomposite alginate hydrogels are quite perspective candidates for 3D printing applications.

We acknowledge funding from the Ministry of Science and Higher Education of the Russian Federation (Agreement No. 075-15-2020-794).

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Self-organization of different-scale structural groups in the Cu/Nb-Ti composite under the action of bundled hydro-extrusion

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[7] National Research Nuclear University MEPhI, Moscow, Russian Federation.
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The samples were obtained using the technology of repetitive package rolling. At the beginning of each cycle, an assembled multilayer package is rolled on a vacuum rolling mill with preheating. Thepackage is welded and turned into a monolithic billet. The monolithic billetis rolled at room temperature to a thin section strip (Fig. 1). In the first cycle, the package is assembled from alternating foils of two or more different metals or alloys. At the subsequent cycles, the package is gathered from multilayer foils after the previous cycle. Thus, an individual foil undergoes a colossal total deformation.

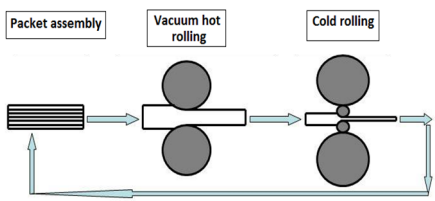

Fig. 1.Obtaining multilayer composites. Scheme of one cycle.

Diffraction patterns were obtained from the studied Cu-NbTi samples in CrKα radiation with a V-filter using a photo-method to analyze the atomic structure of long-range and mesoscopic orders..The photo-method is sensitive to record coherent and incoherent X-

ray scattering, making it possible to examine the details of structural changes in the atomic order.

The newlyobtained material is remarked with an unstressed and relaxed structure. The new material has amodernized composition of elements of various sizes, which form small crystals in the long-rangeand nanoscale layers in the mesoscopic range. The nanoscale layers are fragments from planes with a relatively perfect atomic order (flat clusters), gradually turning into short-range atomic order with a defect structure, intercluster amorphous regions.

In the studied samples, a new structural state appears in the form of periodic fluctuation peaks at the average angles of the diffraction pattern, similar to forming a new metastable nanoscale phase (Fig. 2). The obtained structural state characterizes the composite as a high-strength superconductor.

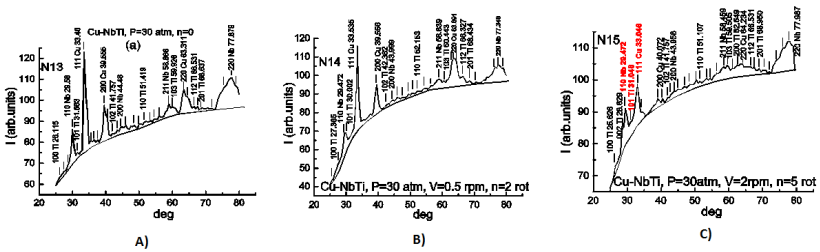

Fig. 2. Diffraction patterns from a Cu-NbTi sample, P = 1 GPa.

The study was performed in the scope of the RO-JINR Projects within the framework of themes FLNP JINR: № 04-4-1140-2020/2022 and № 03-4-1128-2017/2022.

SAXS structural characterization of A8-35 & PMAL-C12 micelles

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Over the past 30 years, amphiphilic polymers (amphipols) have been successfully used in working with membrane proteins [1]. Amphipoles such as A8-35 and PMAL-C12 are used for membrane proteins solubilization.

Amphiphilic polymer A8-35 consists of an acrylic acid polymer (≈35 residues), to the carboxyl groups of which octylamine (z≈9) and isopropylamine (y≈14) are randomly attached (Figure. 1). The average molar mass of A8-35 is 4.3 kDa [2].

The amphiphilic polymer PMAL-C12 is also used as a membrane mimetic for membrane proteins solubilization. The chemical structure of the amphiphilic polymer PMAL-C12, where n≈30, is shown in Figure 2. The molecular weight of PMAL-C12 is approximately 12 kDa. PMAL-C12 is highly negatively charged at neutral pH.

Despite theirs wide applicability, some properties of polymers have not yet been studied, for example, the aggregation number. The study of the free micelles structure could provide important insights for understanding the interaction of these polymers with target membrane proteins.

This research results showed that A8-35 is a monomer with disordered folding and PMAL-C12 has an elongated cylindrical structure with a hydrophobic part facing inward, its aggregation number is ~10. The measurements were carried out on the X-ray instrument Rigaku, MIPT, Dolgoprudny, Russia [3].

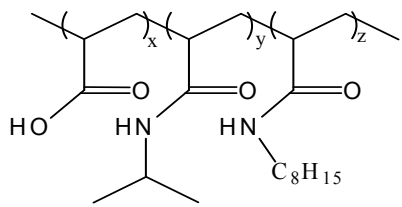

Figure 1. The chemical structure of amphiphilic polymer A8-35

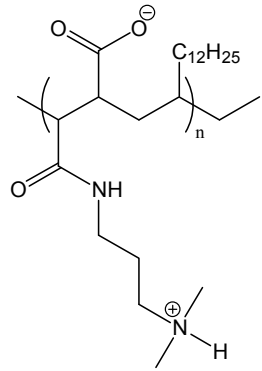

Figure 2. The chemical structure of amphiphilic polymer PMAL-C12

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X-ray fluorescent and magneto-resonant nanostructures based on detonation diamonds

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Synthesis of new combined structures based on detonation nanodiamonds [1] with variable sign of surface potential has been performed using modifying components being medical polymer Polyvinylpyrrolidone (PVP) and Gd-containing organic scintillator (SC) composed of linear alkylbenzene with special additives [2]. The primary complexing of hydrophobic SC and amphiphilic PVP in isopropanol enabled us to prepare the compound based on detonation nanodiamonds (DND Z+) forming stable aqueous dispersions due to repulsion of diamond nanoparticles carrying regulated positive charge on the surface.

Finally, ternary complexes SC-PVP-DND Z+ (approximately equal weight fractions of components) were prepared in a stable form in aqueous media. Structure of the complexes studied by small angle neutron scattering experiments (SANS) exhibited fractal nano-scale ordering of these composites with hydrophilic and hydrophobic components (Fig.1).

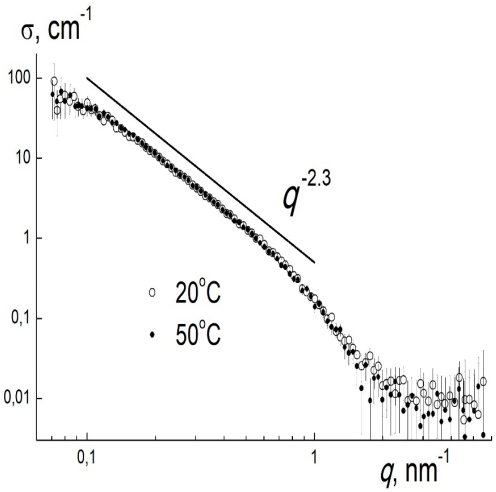

Fig.1. SANS data for ternary complexes SC-PVP-DND Z+ in aqueous medium. Line indicates the scattering cross section's behavior $\sigma \sim 1/q^{2.3}$ vs. momentum transfer for mass fractals of diamond particles.

The modification of diamonds with polymer and scintillator did not destroy normally observed chain-like association of DND Z+ particles in water. The complexes demonstrated branched fractal clusters of same structure initially at 20 °C and by heating up to 50 °C (Fig.1). Structural features of such optically and magnetically active complexes are discussed regarding to their optical absorption and X-ray fluorescent properties (Fig.2) being relevant in biomedical applications.

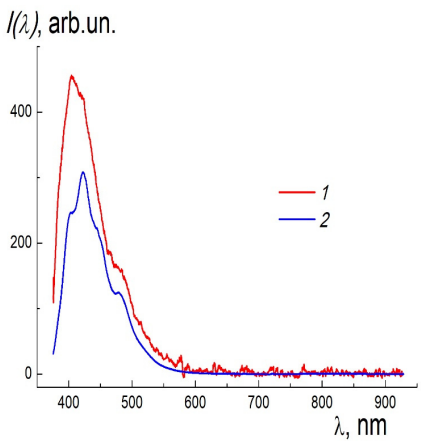

Fig.2. Luminescence of pure LAB-scintillator (1) and complex SC-PVP-DND Z+ (2) excited by X-ray irradiation (wavelength 0.154 nm). The data (1) are reduced by factor 60 for the convenience of presentation.

The complexes have shown the spectrum of luminescence practically in the same band of wavelength ~ 400-500 nm as it was detected for pure scintillator (Fig.2). This spectrum corresponds to Soret band of absorption of medical sensitizer Radachlorin® used in Photodynamic Therapy (PDT).

Thus, it seems appropriate the application of new photoactive complexes in combination with sensitizer to enhance the yield of singlet oxygen in surrounding biological tissues in PDT with the use of X-ray excitation of complexes being able to activate sensitizer.

The work was supported by the Russian Foundation for Basic Researches (gr. No 18-29-19008).

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Magnetostatic equilibrium in concentrated ferrofluids

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Magnetophoresis, that is, the motion of magnetic objects under the action of nonuniform magnetic field, is the physical basis for many applications of magnetic nanoparticles (MNPs) in biotechnology and medicine. Examples of such applications are magnetic cell separation and targeted drug delivery. It is known that the sensitivity of MNPs to the applied gradient field is among main factors determining their suitability for biomedical purposes [1]. In this contribution, we use methods of nonequilibrium statistical mechanics as well as Langevin dynamics simulations to study how the magnetophoretic movement of MNPs in a nonmagnetic viscous medium is affected by interactions between these MNPs (namely, dipole-dipole and Van der Waals interactions). We model a cylindrical microchannel filled with the colloidal suspension of MNPs in a nonmagnetic liquid (i.e., with the "ferrofluid"). A current-carrying linear conductor is placed along the microchannel axis. The system is thermostated. The nonuniform azimuthal field of the current causes the magnetophoretic drift of MNPs in the radial direction. This drift is hindered by the gradient Brownian diffusion. Over time, an equilibrium radial distribution of MNPs will be achieved in the system as the results of competition between magnetophoresis and diffusion. Here the equilibrium radial MNP distribution (as well as the relaxation time required by the system to achieve an equilibrium) is determined for different MNP concentrations and different particle magnetic moments. Simulation results are critically compared with the predictions of ferrofluid masstransfer theories available in the literature.

The work was supported by RFBR (grant No. 19-31-60036).

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Nuclear methods in studies of nanotubes carbon and mineral for thin coatings and membrane layers formation

Lebedev V.T.[1], Kulvelis Yu.V.[1], Torok Gy.[2], Kozlov V.S.[1],
Kamanina N.V.[3], Kononova S.V.[4], Koritkova E.N.[5], Tomchuk A.V.[6]

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Developments in the creation of nano(micro)layers on solid substrates and preparation films with desirable functional properties (conductive, optical, catalytic, providing ionic transport etc.) are realized presently by using various nanoparticles such as fullerenes, detonation diamonds, nanotubes carbon or mineral. Such objects and their layered structures can be characterized by neutron scattering and reflectometry. For example, the latter delivers the information on the formation of the layers of carbon nanotubes (CNT) by their laser ablation and precipitation on substrate (Indium Tin Oxide - ITO) [1]. In reflectivity experiments (JINR, Dubna, Russia) the authors found the profiles of scattering length density for the carbon layer of CNT (length ~ 100 nm) on conducting film covering glass plate (Fig.1). The thickness and the roughness of carbon layers border depended of the applied electric field orienting CNT and on polishing surface by scanning laser beam. We discuss the influence of such treatments on the CNT-coatings. The opportunities of such approaches we extended by a combination with others nuclear methods such as resonant gamma-spectroscopy. The latter allow to study subtle features in atomic coordination of atoms of the elements having special Mössbauer nuclei. Among them, the iron is spread since it play a crucial role as a component of steels and alloys, composite materials, biological tissues, nanostructures such as nanotubes of Mg-Fe-chrysotile [2]. The experimental facility recently created at PNPI (Fig.2) has allowed us to start the experiments on nanodiamonds modified with Eu atoms and determine their valent state at crystalline surface. Further experiments gave the information on subtle features of Fe ions localization in material of nanotubes Mg-Fe-chrysotile as dependent on the content of Fe in them at various amounts of oxides (FeO, Fe_2O_3) in the samples. These nanotubes are considered as

prospective modifiers for diffusive membranes to provide desirable functional characteristics (selectivity for different molecules, permeability).

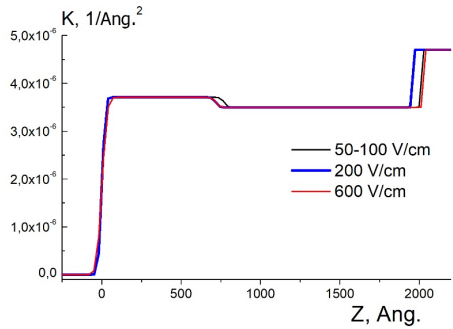

Fig.1. Scattering length density profile for the CNT coating on ITO film deposited on glass. Data for various orienting electric field are given.

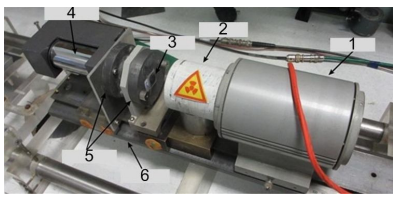

Fig.2. Electrodynamic type Mössbauer spectrometer (PNPI): 1 - gamma radiation source on vibrating frame, 2 – shield, 3 – sample, 4 – photomultiplier tube, 5 – collimators, 6 – optical bench.

Further development of complementary nuclear methods promises a good progress in the studies of new nanostructures materials for wide spectrum of applications.

The work was supported by the Russian Fund for Basic Researches (gr. No 18-29-19008).

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Antioxidant molecule useful in the stabilization of nanoparticles in water suspension

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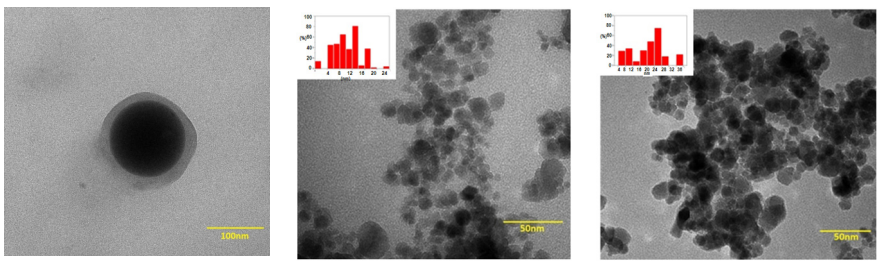
To prepare new biocompatible magnetic nanoparticles the product of co-precipitation method, the magnetite, was coated with gallic acid, a remarkably antioxidant molecule, rather recently considered for core-shell nanostructures preparation. We applied three procedures to obtain gallic acid/magnetite nanoparticles: (i) ferrophase stirring with adequate solution of gallic acid at high temperature, about 80° (M. Szekeres et al., 2005); (ii) room temperature stirring of ferrophase and gallic acid solution; (iii) sonochemical method at room temperature treatment (Wang și colab., 2015).

The final products stability was studied related to the coated ferrophase granularity by means of Transmission Electron Microscopy.



a) b) c)

Fig. 1. TEM images of gallic acid/magnetite nanoparticles Fe_3O_4@GA: a) procedure (iii); b) procedure (i); c) procedure (ii)

In Fig.1. three representative micrographs are shown for the three types of biocompatible magnetic nanoparticles.

Table 1. Physical diameter of gallic acid/magnetite nanoparticles Fe_3O_4@GA

	Fe_3O_4@GA (i)	Fe_3O_4@GA (ii)	Fe_3O_4@GA (iii)
D_{TEM} (nm)	130.0	10.0	19.0

The values of the mean diameter were estimated by analyzing the size of numerous nanoparticle images (Table 1).

According to the requirements of good stability –granularity relationship the sample resulted through the application of protocol (ii) was chosen for further investigations and applications, since the smallest nanoparticles (around 10 nm physicall diameter D_{TEM}) were evidenced.

Other investigations of the physical-chemical properties by corresponding methods were carried out (X-ray diffractometry for crystalinity investigation, Vibrating Sample Magnetometry for magnetic properties, NTA – Nanoparticle Tracking Analysis for hydrodynamical diameter).

The theoretical description of gallic acid structure and properties was carried out (Table 2) by computational means (PM3 method) using Spartan 18 software package.

Table 2. Dipole moment and frontier orbital energies for the gallic acid

Gallic acid	PM3(HyperChem 8.0)	Literature
Dipole moment (D)	1.87	1.8 (Lespade et al., 2010)
Log P	-2.09	-1.3 Andersson et al., 2009)
E_{HOMO} (eV)	-9.310	-9.32 Lu et al., 2006)
E_{LUMO} (eV)	-0.61	-0.61 (Martinez et al., 2003)

The dipole moment and the energies of Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were taken first into consideration as ost important for the gallic acid interaction with metal cations at the Fe_3O_4@GA surface and also with surrounding water. The results were compared with other authors published data being important for the interactions that ensure the colloidal suspension stability. Further investigations are planned by SANS method, at JINR –Dubna to search for complementary data on the nanoparticle properties in fluid suspension.

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Nuclear and optical methods to study irradiated multilayer structures

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Key words*:* Nuclear methods, RBS, ion implantation, Spectroscopic Ellipsometry

Introduction

Multilayer systems such as SiO2/TiO2/Si and TiO2/SiO2/Si have important physical properties, including high dielectric constants, adjustable wide refractive index range, and electro-optic effects.

Experimental

The all samples were implanted with Ne+, Ar+ and Kr+ with the same fluence 3x1016 ions/cm2 and the energy was 250 keV. With the help of Rutherford backscattering spectrometry (RBS) and Spectroscopic Ellipsometry (SE) methods were obtained the depth profiles of elements and the optical properties of the samples.

Results & Discussion

It was noticed that mass of ions increases the dielectric function of all layers have been changed. It was noticed that transient layers between the SiO_2 and TiO_2 are formed. The atomic composition of these layers indicates that they are a mixture of Si, Ti and O elements. The dielectric functions of the study layers. The dielectric function of these layers confirms that the interaction of ions with the atoms of the target creates a layer that describes the EMA model well. The thicknesses of layers determined on the basis of RBS and SE measurements are in good agreement for the samples before and after ion irradiation. The results of these studies indicate that the use of these measurement methods gives precise measurements.

Interfacial effects in polymer-nanoparticle composite films by small-angle scattering methods

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Polymer nanocomposites allow for a large tunability of dielectric permittivity by properly selecting the identity, size, shape, property of filler and by controlling the morphology of polymer matrices, and engineering the interfaces between filler and matrix. The size, shape and concentration of fillers have important effects on dielectric properties. However, the effects of the size and shape of fillers have yet been explored to a sufficient degree [1].

To partially fill the knowledge gap on the influence of nanoparticle filler on the polymer matrix structure, we studied the nanocomposite films prepared by filling the HDPE matrix with two fillers (ZrO_2 and SiO_2) of substantially different properties. Such a set of filler particles enabled us to partially elucidate the relationship between the filler properties and their effect on the HDPE matrix morphology. As we show, the selected nanoparticles alter the structure of HDPE matrix a completely different way.

We studied the interfacial effects in HDPE-nanoparticle composite films using two types of filler particles: nano-ZrO_2 and nano-SiO_2, categorized as ‘inactive’ and ‘active’, respectively. For both fillers, we found that the nanoaggregates are evenly located in the polymer matrix and their surface roughness and fractal character are determined by their initial state in the powders [2].

In the case of nano-ZrO_2 filler the lamellar thickness and crystallinity degree remain unchanged over a broad range of filler concentrations. We propose that in the presence of nano-ZrO_2 filler, the crystallization of HDPE starts in the bulk. Here, the nanoparticles acts as a geometrical hindering factor for growing lamellae. As a result, there are formed zones of reduced polymer density that surround the nanoparticles and are of comparable size (ca. 10 nm). As evidenced by temperature dependent SANS measurements, these zones collapse

at the temperature of 80 °C with simultaneous partial aggregation of the nanoparticles [3]. The phenomenon is driven by polymer chain displacements related to the α-relaxation process [4].

Silica nanoparticles exert a completely different impact on the crystallization of HDPE under rapid quenching conditions. Here we found that both the lamellar thickness and the degree of crystallinity increase with increasing the filler loading. Based on this, we propose that nano-SiO_2 particles are 'active' in HDPE crystallization, supposedly acting as nucleation centers for lamellae growth [5]. Based on SAXS measurements, the ordering of the lamellae is disrupted even at a filler content of a few percent. Since the crystallization starts on the particles surface, not in the bulk, no cavity zones are present. The changes of SANS curves at different temperatures in range from 20 °C to 120 °C are not visible also.

This different behavior of both fillers is expected to lead to different mechanical and dielectric properties of the nanocomposites and will be the subject of our further study.

Acknowledgement

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Computer simulations of a ferromagnetic inclusion in a polymer matrix

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Magnetoactive elastomers (MAEs) are polymer composites that consist of a polymer matrix and ferromagnetic filler particles dispersed in it. Due to the presence of ferromagnetic filler in the material it is possible to influence its properties via an external magnetic field. Magnetized filler particles interact with each other and with the external field and rearrange inside the matrix, if it is possible. Thus, mechanical and electromagnetic properties of MAEs can be controlled externally.

The aim of this work is to study the filler restructuring in MAEs using theoretical methods and computer simulations. Here the problem of a ferromagnetic inclusion in a polymer matrix is considered. Object of an arbitrary shape is placed in a hyperelastic medium. The medium's response to the movement of the object caused by magnetic field is then studied using finite element method. This object can represent a single particle or a cluster of tightly packed particles moving as a whole. The shape of the object is chosen primarily to be that of an ellipsoid with varying anisometry ratio.

Mechanical response (stress-strain) and the energy of a cell containing the ellipsoid are calculated for different filler concentrations, shapes (disk-like and needle-like ellipsoids), anisometry ratios and magnetic fields. Both linear and non-linear elasticity are considered. Various mechanical loads are prescribed to the cell corresponding to different boundary conditions. For the linear regime effective elastic modulus of the cell and the linear regime limits are calculated as well.

The obtained results will later be used in simulations of ferromagnetic inclusion systems and ensembles.

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Structural ordering of magnetic and non-magnetic nanoparticles in aqueous media by SANS

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Current interest in colloidal systems containing magnetic and nonmagnetic nanoparticles (NPs), such as magnetic fluids, is due to an effective combination of properties and features at nanoscale affecting on their bulk state, which is useful in various industrial technologies and biomedical applications [1-3]. Thus, for example, the combination of fluidity and magnetism is important for biomedical applications [4]. Colloidal nanoparticles (including magnetic NPs) intended for these purposes should have as narrow size distribution as possible, be chemically stable, non-toxic, and at the same time demonstrate superparamagnetic properties. For effective use, colloidal NPs ought to have controlled size and, as far as possible, be resistant to formation of large aggregates. Colloidal aggregation cannot be avoided completely in water-based magnetic fluids [5]. The issue of aggregation becomes especially important in biorelevant solutions, which are naturally water-based.

The reason for aggregation in an aqueous medium is the dominance of the energy of interaction between particles over the energy of thermal motion in the medium that is especially pronounced for magnetic NPs. This work considers structural studies of aqueous magnetic fluids and aqueous dispersions with nonmagnetic nanoparticles basing par excellence on small-angle neutron scattering techniques as powerful tool in condensed matter science.

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Specifics of fullerenes cluster formation in polar/nonpolar solvent mixture

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Fullerene is a molecular compound consisting of carbon atoms. Along with other allotropic forms of carbon, such as diamond or graphite, fullerenes are the first form, soluble in a wide variety of organic and inorganic solvents. Fullerenes are widely used in various fields, including optics, electronics and medicine [1-3].

For these purposes, the production of liquid solutions of fullerenes is necessary [4]. Despite of a wide application of fullerene solutions, the processes of their aggregation in solvents and the processes of interaction between fullerenes and solvents are still unclear [5].

In the present work the structure of fullerenes C_{60} and C_{70} in polar and non-polar solvent mixtures was investigated. Toluene and N-methyl-2-pyrrolidone were chosen as solvents. To carry out these tasks the methods of small-angle neutron scattering, small-angle X-ray scattering, dynamic light scattering and UV-vis spectroscopy were used.

As a result, the correlation was observed between the fullerene aggregates formation and a volume fraction of the nonpolar solvent toluene. The dependence of the structural state of fullerene C_{70} on the polarity of the liquid medium was studied; an increase in the volume fraction of the polar solvent toluene above the threshold value of 70% led to the destruction of the existing large aggregates and the reorganization of the clusters. The obtained data were analyzed in comparison with the previous results for the similar colloidal systems with fullerene C_{60}.

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Structural studies of asolectin liposomes by small-angle scattering

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Liposomes are a model membrane system of cellular organelles and cells, which is also can be used for functional tests of membrane proteins. In addition, liposomes can be used as drag-delivery systems[1]. Structural studies of liposomes are an important task that will advance the understanding of the physical properties of these model systems.

In this study, liposomes from asolectin were studied by small-angle X-ray scattering[2] under different condition. The gyration radius in the infinite plane approximation(Rt) and consequently the number of bilayers were calculated for each samples. The dependence of this parameter on various conditions, such as the pH of the medium and the concentration of asolectin in the solution, was obtained.

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Magnetophoresis in magnetic fluids in inhomogeneous magnetic fields

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The process of magnetophoresis in a thin layer of MF under prolonged exposure to inhomogeneous MP of several configurations is studied. In axisymmetric magnetic systems with the use of unipolar permanent magnets, capable of creating a magnetic field with a strength of 500 kA/m in a sufficiently extended region, the course of the magnetophoresis process in MF samples with different microstructures is experimentally studied. The experiment was carried out using the method of photofixing the dynamics of the interphase boundary in a flat thin optically transparent cell filled with MF, from the bottom of which a controlled illuminator was fixed. In an experiment on a long-term (~30 days) study of the process of magnetophoresis in MF in the magnetic field, it was found that for a sample of MF containing larger MNPs (d~15 nm), the process of magnetophoresis proceeds 5 times faster than in a sample of MF with smaller MNPs (d~7 nm). In the case of the monodisperse approximation, without taking into account the diffusion processes, an expression is obtained for the diameter of the magnetic particles involved in the magnetophoresis process, on the basis of which, according to the experimental data, the dependences of the size of the MNP on the exposure time are constructed, shown in Figure 1.

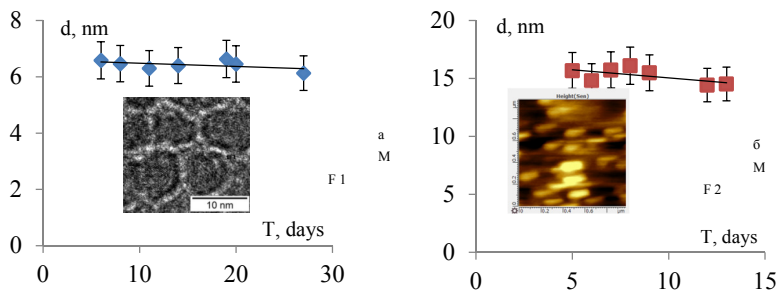

Figure 1. The dependence of the average diameter of the MNP MF, in comparison with the data obtained by TEM and AFM

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Structuring of magnetic nanoparticles inside the membrane of an elongated polymersome

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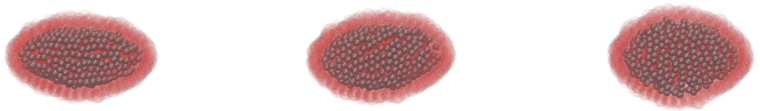
Development of intelligent containers for remotely guided intracellular drug delivery is one of the most relevant tasks of modern nanosurgery. A possible solution is synthesis of magnetosensitive vesicles (polymersomes) [1]. The inner space of these capsules offers a submicron reservoir that might be filled with therapeutic or/and diagnostic content, whereas the outer membrane (wall) is formed by a double layer of an amphiphilic polymer inside which magnetic nanoparticles (MNPs) are enclosed. The developed methods of synthesis enable one to produce polymersomes with a wide range of morphologies and structures. In particular, the amphiphilic macromolecules, when being assembled in layers, could be linked in such a way that the resulting capsules are non-spherical. Such polymersomes, prolate in particular, are considered as promising candidates for creating nanodevices capable of penetrating cellular membrane, i.e., provide tools for cellular surgery. An external AC field by inducing alternating motion of the nanoparticles produces oscillations of the overall polymersome shape. Due to that, the capsule becomes a nanoscale source of pulsation pressure that can be effectively used in the cell mechanobiology.

In the presented work, by the means of coarse-grained molecular dynamics simulations the quasistatic response of prolate magnetic polymersomes to an applied field is studied. The modelling is performed using ESPResSo [2]. The real polymersome is schematized as a closed layered particulated structure consisting of the beads (coarse grains) of two types bonded by a set of interparticle potentials. The outer and inner shells constructed of polymeric (non-magnetic) beads, imitate the layers of the amphiphilic membrane; the MNPs are confined between those layers. The beads of each membrane are connected by Hookean springs to tune the stretching and bending properties of the shell as well as its thickness. The MNPs are assumed to be soft spheres interacting with each other via magnetic dipolar potential. Soft repulsion is assigned also to the interaction between the MNPs and polymeric beads in order to prevent the nanoparticles from migration neither inside the polymersome or outside the membrane. All the system is placed in a bath with constant temperature (Langevin thermostat) and subjected to an external magnetic field.

The above-described computational experiment is carried out under a progressively increasing (in a quasistatic way) magnetic field. Several orientations of the latter with respect to the major axis of the ellipsoid-like polymersome were considered, see Figure 1. The results of statistical analysis of spatial rearrangements of the MNPs under the action of the field would be presented in the talk.



a) b) c)

Figure 1. Snapshots of the final magnetized configuration of an elongated magnetosensitive vesicle: a) magnetic field is directed along long axis of the vesicle, b) magnetic field is directed at an angle of 45 degrees to the long axis of the vesicle, c) magnetic field is directed along short axis of vesicle.

The study was supported by a grant from the Russian Science Foundation (project No. 20-71-00045).

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Bovine serum albumin binding impact of the biogenic ferrihydrite nanoparticles produced by *Klebsiella oxytoca*

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Bovine serum albumin (BSA) acts as a carrier for many ligands such as flavonoids, hormones, and nanoparticles, including biogenic nanoparticles. The best medium for the biosynthesis of iron nanoparticles, such as ferrihydrite nanoparticles, is bacteria. The ferrihydrite nanoparticles used in this study were synthesized by Klebsiella Oxytoka bacteria in different conditions (dark, light, frozen). The morphology and the structure of the particles is characterized by means of scanning electron microscopy (SEM) and small-angle X-ray (SAXS) methods. In order to evaluate the binding mechanism between the biogenic nanoparticles and BSA, we used UV-Vis spectroscopy, fluorescence, fluorescence resonance energy transfer (FRET), and molecular docking.

The dispersion of the ferrihydrite nanoparticles was investigated by UV-Vis spectroscopy. The darkness conditions are favorable for the increase of the absorbance, suggesting that in darkness, the organic matter could be attached strongly to the surface of ferrihydrite nanoparticles. All biogenic ferrihydrite nanoparticles bind to BSA at one site, with very weak affinity constants, by a static process, confirmed also by the FRET efficiency and the distance between the two partners. The thermal stability of BSA was favored in the presence of biogenic ferrihydrite nanoparticles. Following molecular docking, the best position of the ferrihydrite in the protein binding site determined, and spectroscopic results were confirmed.

These results can be a starting point for the use of the biogenic ferrihydrite nanoparticles in medical applications targeting processes such as circulation, distribution, biocompatibility bioavailability.

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The influence of ferrihydrite nanoparticles on human serum albumin corona

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Human serum albumin (HSA) binds and carries a very large variety of small molecules - flavonoids, ions, vitamins, and nanoparticles such as iron oxide nanoparticles. In this study, we used chemical ferrihydrite nanoparticles (Fh-NPs) simple and doped with Co and Cu due to their physicochemical properties [1, 2]. To analyze the formation and organization of HSA corona molecules around nanoparticles and to evaluate the morphology and particle size, we used Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). Molecular docking studies were used in order to determine the probable location of the ferrihydrite in the HSA structure. In order to establish the thermal stability of the protein alone and in complex with the nanoparticles, fluorimetry was used by analyzing the behavior of Trp-214 residue from HSA and the denaturation temperature was determined.

SEM and AFM experiments revealed the dimensions of Fh-NPs and the organization of HSA molecules around Fh-NPs, in a fairly regular corona. The average diameter of Fh-NPs coated with HSA corona was ≈150 nm for simple Fh-NPs, ≈100 nm for Co-Fh-NPs, and ≈12 nm for Cu-Fh-NPs. The molecular docking simulation shows that ferrihydrite is binding to the metal-binding site of HSA, with a low affinity. Thermal denaturation of HSA alone and in complex with Fh-NPs produces intermediate states and the temperature of transition is almost the same for all complexes excepting HSA-Co-Fh-NPs sample.

The biophysical effect of Fh-NPs on serum proteins is the first step in their use in biological applications as hyperthermia, drug targeting, and diagnostic applications (nuclear magnetic resonance imaging).

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The network of entangled surfactant wormlike micelles with the embedded halloysite nanotubes

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Ionic surfactants with a relatively long tail are known to be aggregated in long cylindrical micelles in the presence of salt in an aqueous medium. Such wormlike micelles entangled with each other form a three-dimensional viscoelastic network in the solution. The characteristics of these properties, such as the elastic modulus, viscosity, and relaxation time, are determined by the shape and length of the micelles and vary depending on the salt concentration, surfactant concentration, pH of the medium, and temperature [1,2]. Therefore, such micelles are called living polymers. Viscoelastic surfactant solutions are widely used in oil production, household chemicals, cosmetics [3]. One of the disadvantages of such solutions is the relatively low mechanical properties. There are a number of approaches to solve this problem by adding cosurfactants or polymers of different architectures [4]. One of the new approaches developed in the literature and in our laboratory is the addition of nanoparticles [5]. Nanoparticles can be embedded in a network of entangled micelles acting as physical cross-links between the micelles. This interaction is possible due to the attachment of the micelles end parts to the surfactant layer on the surface of the nanoparticles. Since the number of energetically unprofitable ends in the system decreases, this is favorably [5]. In this paper, network of wormlike micelles of cationic surfactants in the presence of salt and halloysite nanotubes are investigated [6].

Conditions for the formation of linear and branched wormlike micelles by varying the concentration of surfactant and salt were determined. The dependencies of the rheological properties on the composition of the solution were obtained. The stability conditions of suspensions in depend on the charge value of the nanotubes are obtained. It is shown that the addition of nanotubes to the network of wormlike micelles leads to an increase of the relaxation time, the elastic response region of the system, and the viscosity of the system, the value of the last one changing by 2 orders of magnitude under certain conditions.

Thus, viscoelastic suspensions of surfactant wormlike micelles and nanotubes of natural clay of halloysite were prepared and studied. It is found that the addition of nanotubes increases the viscosity and relaxation time by orders of magnitude, but weakly

affects the elastic modulus of the system. It is shown that the change in properties occurs due to the junction of wormlike micelle to nanotubes, and the binding force depends on the charge of the nanotube surface.

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Phospholipid phase transition at increased hydrostatic pressure: Repeat distance and bilayer thickness

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Despite numerous investigation of the lipid membranes, the main issues of the hierarchical organization and morphology of lipid systems with temperature and pressure changes remain the subject of wide scientific discussion. The so-called main lipid membrane phase transition has features of both the first and the second order transitions. Moreover, the effect of anomalous swelling and the corresponding balance of forces (van der Waals, Helfrich and entropy) cause scientific debate [1, 2].

In our work, we consider the influence of hydrostatic pressure and temperature variation on unilamellar lipid membranes thickness and multilamellar membranes repeat distance. The small angle neutron scattering experiments were carried out at FLNP, JINR on the YuMO spectrometer with a two-detector system using the time-of-flight technique [3]. The high pressure setup was used in the configuration described in [4]. The SANS curves for heavy water dispersion of DMPC unilamellar lipid vesicles under pressure is shown in Figure 1.

The pressure and temperature variation in the corresponding range leads to a change in the lipid membrane phase state: with an increase in hydrostatic pressure, lipids pass from the liquid phase to the gel phase, and with an increase in temperature, lipid membranes from the gel phase pass into the liquid phase. During the transition from the gel phase to the liquid phase, the thickness of the lipid bilayer decreases, and the area per lipid molecule increases [1, 5]. Experiments carried out under high hydrostatic pressure show that there are changes in the thicknesses of the bilayer, the water intermembrane layer and the multilamellar membranes repeat distance.

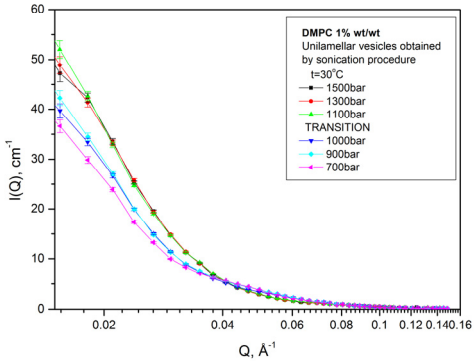

Figure 1. SANS curves for DMPC 1% wt/wt unilamellar vesicles D2O dispersion under high hydrostatic pressure. The transition is observed in range between 1000 and 1100 bars.

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Behavior of water droplets in a magnetic liquid in an inhomogeneous magnetic field

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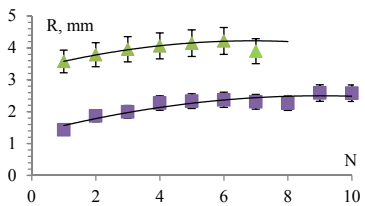
An experimental setup for high-speed video recording of the dynamics of water droplets in the MF in the magnetic field of an annular magnet is described. The experiment consisted in the following: the Hele-Shaw cell is filled with MF, an annular magnet is brought coaxially to the cell from below with the help of a mechatronic actuator, and a drop of non-magnetic liquid MF is captured at a certain distance between the surface of the MF and the upper plane of the annular magnet. When the magnet is further lowered, a drop of non-magnetic liquid is pressed to the bottom by an inhomogeneous magnetic field, after which small drops are separated [1]. Archimedes force on the dynamics of drops. An experiment on video recording of the dynamics of the separation of droplets from the water volume held in the region of the change in the sign of the magnetic field gradient in a magnetic liquid was carried out, on the basis of which the sizes of water droplets for different concentrations of the magnetic liquid were determined. The figure shows the dependence of the size of small droplets that break away from the main volume of a non-magnetic liquid on the ordinal number. A theoretical estimate of the balance of forces for the separation of a non-magnetic drop in a magnetic liquid is made.



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The volumetric adsorption hydroelectric transducer for a new alternative energy

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The relevant task at the moment is the studying new size effects and possibility of their practical using in modern alternative energy technologies. The scientific and practical interest are the technologies of adsorption air conditioning, which make it possible to stabilize the temperature in a room through the thermodynamics of adsorption-desorption processes [1,2,3]. The development of laboratory layout of such devices was the goal of this work.

The experimental samples of functional media for a new alternative energy sources based on adsorption induced nonequilibrium physical-chemical processes (β-α phase structural transformation) in the system of zirconium dioxide nanoparticles was made [4,5] (fig. 1).

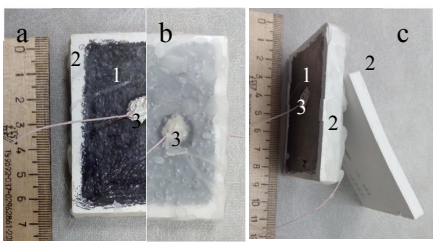

Fig. 1. Chemoelectronic converter: from the adsorbing (b) and waterproofed (c) sides surfaces; view from the top (c), where: 1– carbon electrodes (located on both sides of the converter), 2- working fluid - porous block of YSZ - nanopowder; 3- silver-glue contact.

Atmospheric humidity was used as the adsorbent (energy source) whereas the wide band gap ZrO_2–based nanoparticles of 7.5 nm - as the absorber. The surface of a nanoparticle /

gas formed a functional heterojunction. The source of uncompensated charge carriers was the adsorption front, which moved from the open surface (Fig. 1, a) to the waterproofed surface of the sample (Fig. 1, b). Measuring cell is shown on Fig. 2..

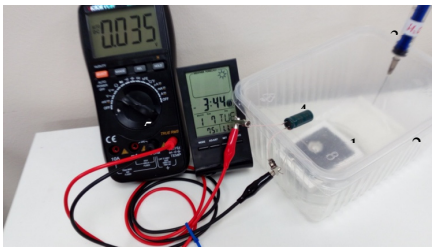

Fig. 2. Measuring cell, where: 1 - sample of a chemo-electric converter; 2- humid air chamber; 3- syringe with distilled water; 4– electric capacitor 2200mkf x 6V.

Test device with specific surface area of heterojunction S_{BET} = 128 m^2/g produced over W = 260 mkW/kg power density on the capacitor electrical load of 2200 mkF at relative humidity of 90%. The energy that the capacitor stored during the working cycle is sufficient for reliable deflection of the staple of an electromechanical microammeter. Thus, obtained device indirectly demonstrate the possibility of a new renewable energy source creation.

The study was performed in the scope of the H2020/MSCA/RISE/SSHARE number 871284 and the RO-JINR Projects within the framework of themes FLNP JINR: 04-4-1143-2021/2025 and 03-4-1128-2017/2022.

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Small-angle scattering structural studies of recombinant apoferritins from various organisms

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Ferritin is one of the main iron-containing proteins in the organism. Its main function is considered to be iron transport and storage. One protein molecule may contain up to 4500 ions of this microelement in the form of ferrihydrite [1]. Protein without iron is called apoferritin. Concentration of ferritin in the human blood increases with age, which indicates the participation of this protein in the aging process of the body [2].

Recombinant apoferritins from organisms *Helicobacter pylori* and *Escherichia coli* were obtained. Proteins include His-Tag for Nickel-NTA and SEC purification. Proteins were expressed, purified and studied by small-angle X-ray scattering (SAXS) methods. The study of the structural properties by the SAXS method was carried out on the Rigaku [3].

Obtained data confirm the structural similarity of apoferritins from different organisms. The form factor of apoferritins obtained via SAXS method is in a good agreement with the data of high-resolution structures from the Protein Data Bank (PDB) library and literature data [4, 5].

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Application of the Rutherford backscattering method in powder nanotechnology

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Rutherford Backscattering Spectrometry (RBS) is an ion scattering technique used for compositional thin film that are less than 1μm thick analysis. During an RBS analysis, high-energy He^{2+} ions with energies in the region from several hundred kiloelectron-volts to 2 - 3 MeV are directed onto the sample and the energy distribution and yield of the backscattered He^{2+} ions at a given angle is measured. Since the backscattering cross section for each element is known it is possible to obtain a quantitative compositional depth profile from the RBS spectrum obtained.

The capabilities of this method can be significantly expanded. In particular, the method can be used in powder nanotechnology to study elemental composition in microscopically small objects.

The application of methods based on Rutherford Backscattering Spectrometry is extremely interesting for adsorption energy devices, in particular, these methods can be used with maximum efficiency for various chemoelectronic converters.

A unique opportunity is to study the elemental surface of adsorbates on the surface phase separation in functional nanostructured layers.

For this reason, the preparation of planar-distributed chemoelectronic converters and the study of the elemental composition of adsorbates using the Rutherford Backscattering Spectrometry technique was the purpose for the investigation.

The tasks of this study included: development and optimization of the technology for producing planar chemoelectronic converters a functional layer in the form of rounded drops containing monodisperse nanosized (7.5 μm) particles of a solid solution of the ZrO_2 system - 3 mol% Y_2O_3 (YSZ) in the PVA polymer matrix, study of the theoretical characteristics of the obtained chemoelectronic converters [1], study of the elemental

composition of the obtained chemoelectronic converters using Rutherford Backscattering Spectrometry.

The atomic and chemical composition of these layers has been studied using nuclear and atomic methods.

The thickness of the oxide layers was found to be approximately the same for all implanted samples. These values were determined on the basis of Rutherford Backscattering Spectrometry and nuclear reactions (RBS/NR).

The study was performed in the scope of the Poland-JINR and the RO-JINR Projects within the framework of themes FLNP JINR: 04-4-1140-2020/2022, 04-4-1143-2021/2025, and 03-4-1128-2017/2022.

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The effect of a polarizing magnetic field on the dynamic properties and of the specific absorption rate of ferrofluids in the microwave range

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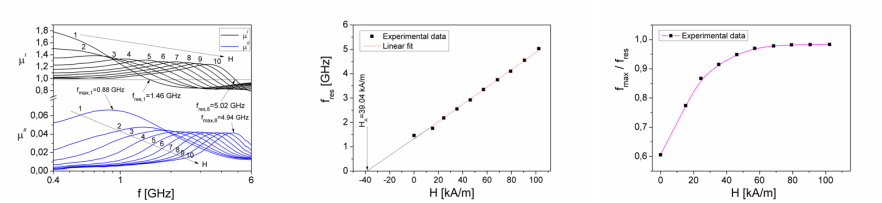
The complex magnetic permeability, $\mu(f, H)=\mu'(f, H)-i\mu''(f, H)$, of a kerosene-based ferrofluid sample with magnetite particles, in microwave range, from 0.4 GHz to 6 GHz, and for various values of polarizing magnetic field H over the range 0 to 102 kA/m, was measured [1, 2]. In this frequency range, both the ferromagnetic resonance at a f_{res} frequency and the corresponding maximum absorption at a f_{max} frequency were highlighted, frequencies that move to higher values by increasing the H field (Fig. 1) [3].



a) b) c)

Figure 1. (a) The plot of the complex permeability of ferrofluid sample as a function of frequency, f and at different values of polarizing field, H; (b) dependence of $f_{res}(H)$; (c) dependence of the ratio f_{max}/f_{res} (H)

Starting from the Landau - Lifshitz equation [4] it can be shown that in a strong polarizing field (i.e. $H > H_A$) [3, 5], the resonance condition is written as:

$$2\pi f_{res} = \gamma\left(H + H_A\right) \tag{1}$$

The gyromagnetic ratio of particle, γ can be theoretically computed [3] with the relation:

$$\gamma = g\gamma_e\mu_0\left(1+\alpha^2\right)^{1/2} \tag{2}$$

In equation (2), g is the spectroscopic splitting factor and $\gamma_e = 8.791\cdot10^{10}$ $s^{-1}T^{-1}$, is the electronic gyromagnetic ratio [5, 6]. As demonstrated in [3], the damping parameter of the Landau–Lifshitz equation, α, in strong polarizing field ($H > H_A$) is given by the relation:

$$\alpha = \sqrt{\frac{1-(f_{\max}/f_{res})^2}{1+(f_{\max}/f_{res})^2}} \tag{3}$$

From the H dependence of both the f_{res} frequency (Fig. 1 b) and the f_{max}/f_{res} ratio (Fig. 1 c), and Eqs (1), (2) and (3), we determined the anisotropy field, H_A, the anisotropy constant K_{eff}, of nanoparticles, the gyromagnetic ratio, (γ), the damping parameter (α), the spectroscopic splitting factor (g) and the internal magnetic viscosity (η_m). Also, the theoretical Neel relaxation time τ_N, based on resonance measurements, was estimated, taking into account that the ratio $\sigma = (K_{eff}V_m/kT) > 2$. The obtained values of these parameters are listed in Table 1.

Table 1. The dynamic parameters of nanoparticles from ferrofluid in microwave field

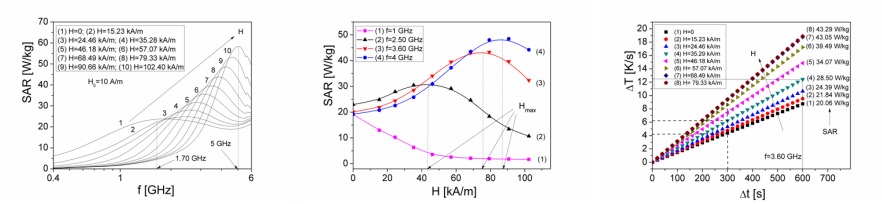
H_A [kA/m]	K_{eff} [J/m^3]	γ [s^{-1}A^{-1}m]	α	g	η_m [Nsm^{-2}]	σ	τ_N [ns]
39.04	$1.17\cdot10^4$	$2.23\cdot10^5$	0.114	2.007	$1.95\cdot10^{-6}$	2.024	5.07

From the magnetic permeability measurements, the specific absorption rate (SAR) were determined (Fig. 2 a), using a new equation for the calculation of the SAR of ferrofluids:

$$SAR = c\frac{\Delta T}{\Delta t} = \frac{1}{(1-\varphi)\rho_L + \varphi\rho_S} p_m = \frac{1}{\rho_F} p_m \tag{4}$$

where, p_m represents the specific magnetic power loss from the ferrofluid [7, 8]; φ is the volume fraction of the solid phase. Equation (4) differs from that used by most authors who do not take into account the density of the ferrofluid ρ_F, but only the density of the solid particles dispersed ρ_S [9, 10] The SAR presents a maximum at a value H_{max}, which moves to higher values by increasing the frequency f, which are found in the range of ferromagnetic resonance frequencies (Fig. 2 b).

As can be observed from Fig. 2 c), for a polarizing magnetic field, H=35.29 kA/m corresponding of frequency 3.60 GHz, at an application time of the variable electromagnetic field of Δt=300 s, the increase in temperature is, ΔT=6.20 K, while at H=0, for the same time duration (300 s), the increase in temperature is only 4.01 K. This result correlates with the fact that the specific absorption rate (SAR) increases from 20.06 W/kg (at H=0) to 28.50 W/kg (H=35.29 kA/m), as observed in Fig. 2c).



(a) (b) (c)

Figure 2. (a) The frequency dependence and magnetic field of the SAR of the ferrofluid; (b) The polarizing magnetic field dependence of the SAR at different frequency *f* of microwave field; (c) The time dependence of the heating rate $\Delta T / \Delta t$ at a constant frequency *3.6 GHz* at different values of the polarizing magnetic field

This obtained results provide an opportunity to control the specific absorption rate and the increase in temperature ΔT, through the field *H*, applied of ferrofluid, with applications in the cancer treatment by magnetic hyperthermia. Also, knowledge of the magnetic parameters of nanoparticles from ferrofluid, is usefull in the design and manufacture of some microwave devices.

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Iron oxide nanoparticles coated with silica for nucleic acids separation

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The development of effective methods for individual cells or molecules separation is the important and perspective task of laboratory diagnostics today. It allows to investigate selectively separate components of complex biological samples, reducing nonspecific signals from impurities and thereby significantly increasing the sensitivity and specificity of the analysis. The use of magnetic nanoparticles for the separation of biological objects (molecules, cells) has become widespread due to the ease of use, relative safety in combination with the ability to obtain a pure product, and the possibility of automating the process. Magnetic separation is one of the most specific and convenient methods. But the development of nanoparticles requires special attention to the composition in order to combine the beneficial properties of the nanoparticle with its safety for the cell. The aim of this study was to synthesize and investigate magnetic nanocomposites of iron oxide for the following functionalization for nucleic acids separation.

The magnetic particles were prepared by coprecipitation from a solution of $FeCl_3$ and $FeCl_2$ salts in a molar ratio of 2:1 at room temperature. With constant stirring, an NH_4OH solution (25%) was injected into the solution of iron salts until pH = 10 was reached. At the end of the reaction, the magnetic nanoparticles were collected using a magnet and washed several times in distilled water until pH = 7.0. To use nanoparticles in magnetic separation of DNA, the surface of the particles was modified with silica using tetraethoxysilane (TEOS). The nanoparticles were studied by transmission electron microscopy, IR spectroscopy, magnetometry. The studies were carried out on the equipment of the Krasnoyarsk Regional Center of Research Equipment of Federal Research Center «Krasnoyarsk Science Center SB RAS».

Figure 1 shows the FTIR spectrum of magnetic nanoparticles coated with silica. Analysis of IR spectra showed the presence of Fe-O bonds (~590 cm^{-1}). The peaks of strong stretching vibrations of siloxane groups Si-O (~ 1090 cm^{-1}) and silanol groups Si-OH (~

800 and ~ 960 cm^{-1}) prove the formation of a silicon oxide shell on the surface of a nanoparticle. The stretching vibration ν-OH forms an intense band in the region of 3200-3600 cm^{-1}.

The magnetization curves measured in the range from -15 to 15 kOe are symmetric about the origin and contain a reversible part as well as an irreversible part - a hysteresis loop (Fig. 2). The coercive force, remanent magnetization, and magnetization in a field of 15 kOe decrease with increasing temperature.

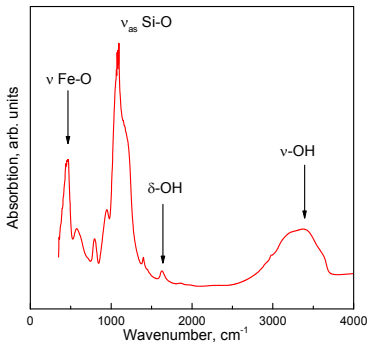

Fig.1. Room-temperature FTIR spectrum of Fe_3O_4@SiO_2

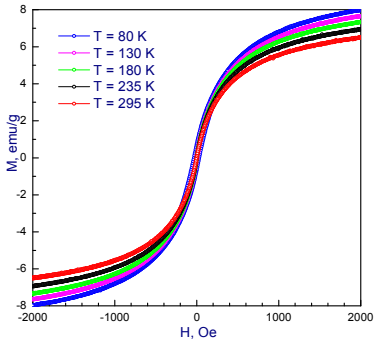

Fig.2. Hysteresis loops

Isolation of DNA from blood cells with the help of magnetic particles has been carried out. A commercial kit containing a silicate sorbent for DNA was used as a control. The amount and quality of DNA using magnetic nanoparticles were comparable to the amount isolated using a silicate sorbent.

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Formation of apoferritin dimers and trimers via hydrophobic 4-fold channel contacts: SEC-SAXS investigation

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Apoferritin is a complex of 24 protomer molecules. The apoferritin protomer has a mass of ~ 20 kDa; it forms dimers, which are then assembled into a rhombododecahedron with 12 faces and 14 vertices (8 triangular and 6 tetrahedral). The final 24-mer has the shape of a spherical shell, the inner cavity of which is intended for storing iron oxide. There are eight 3-fold and six 4-fold channels through which iron enters the core.

In this work, the structure of apoferritin oligomers was studied using SEC-SAXS (size-exclusion chromatography coupled with small-angle X-ray scattering). The measurements were performed on the BM29 beamline, ESRF, Grenoble, France [1]. SEC-SAXS profile for apoferritin has two peaks (Fig. 1). Comparison parameters R_g and D_{MAX} with the data from [2] shows that peak (A) corresponds to the apoferritin monomers, peak (B) corresponds the trimers possibly mixed with monomers and dimers.

For apoferritin trimers, the mutual arrangement of monomers depends on the position of protein-protein contacts. The interconnected centers of mass of monomers in the apoferritin trimer form an isosceles triangle. The type of molecular interaction determines the values that the vertex angle of this triangle can take. If 4-fold channels are involved in the formation of oligomers, then the vertex angle can take three values of 90° and 180°; if 3-fold channels are involved, values of 70.5° and 109.5° are possible; and if 2-fold channels are involved, 60°, 120° and 180° are possible.

Because the apoferritin monomer has a shape close to spherically symmetric, the ratio of the SAXS curve obtained for a mixture of monimers / dimers / trimers to the curve from monomers (shown in Figure 2) can be approximated by the following formula:

$$\frac{I_{mix}(q)/c_{mix}}{I_{mon}(q)/c_{mon}} = 1 + \alpha_2 \frac{\sin qL}{qL} + \sum_j \alpha_3^j \left(\frac{\sin\left(2qL \sin\frac{\varphi^j}{2}\right)}{qL \sin\frac{\varphi^j}{2}} + 4 \int_0^1 J_0\left(qL \cos\frac{\varphi^j}{2}\sqrt{1-x^2}\right) \cos\frac{qLx \sin\frac{\varphi^j}{2}}{2} dx \right)$$

where α_2 and α_3^j are fractions of dimers and trimers with vertex angles φ^j, respectively.

Using coefficients α_2 and α_3^j and c_{mon}/c_{mix} ratio as fit parameters, the distribution of the mixture components was calculated (see Fig. 2). The dominant components of the mixture corresponding to the peak (B) are apoferritin monomers and its trimers corresponding to an angle of 90°. The fact that the vertex angle in the trimers is 90° indicates that 4-fold channels are involved into the formation of oligomers. Comparison of the amino acid composition in the region of 3-fold and 4-fold channels shows that the 3-fold channels are mainly hydrophilic, and the 4-fold channels are hydrophobic. This result is in good agreement with the conclusions of [3], in which it was suggested that the mechanism of apoferritin dimerization is associated with a hydrophobic interaction.

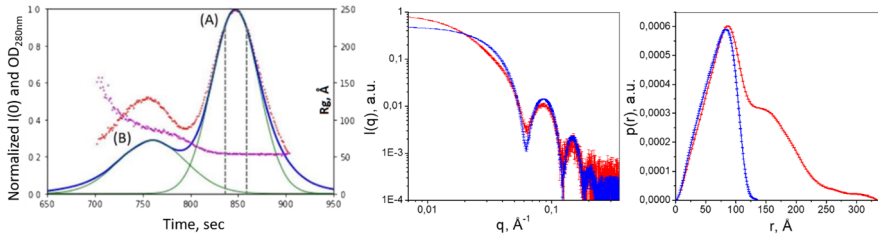

Figure 1. SEC-SAXS profile of apoferritin (*Left*), I(q) and p(r) dependencies (*Middle* and *Right*, respectively) corresponding to peak fractions (A) (blue curves) and (B) (red curves).

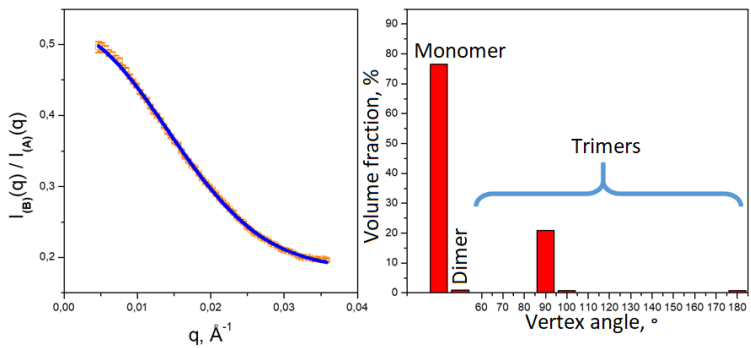

Figure 2. Experimental intensity ratio I(B)(q)/I(A)(q) (orange points) and corresponding fit (blue curve) (Left) and histogram of volume fractions of apoferritin monomers, dimers and trimers (Right).

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Gaussian curvature map on a real surface of lipid cubic phases as a model system for membrane protein crystallization processes

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Lipid cubic phases (LCPs) is a membrane-mimicking system that is useful for membrane protein crystallization due to its' unique properties and close-to-native conditions. One of the features of LCPs is 3D infinite periodicity which allows lateral diffusion of membrane proteins, thus creating layers of proteins consequently triggering 3D-crystal growth [1].

In this work we studied how the Gaussian curvature K(x,y,z) is distributed along the surface of the LCPs with different group symmetries (Im3m, Pn3m, Ia3d) and found that it creates areas with low values of K(x,y,z) meaning the low free energy creating by membrane curvature. The Gaussian curvature K(x,y,z) equal[2]

$$K(x,y,z) = \Big\{ [\, f_z(f_{xx}f_z - 2f_xf_{xz}) + f_x^2 f_{zz}] \times [\, f_z(f_{yy}f_z - 2f_yf_{yz}) + f_y^2 f_{zz}] - \big(f_z(-f_xf_{yz} + f_{xy}f_z - f_{xz}f_y) + f_xf_yf_{zz}\big)^2 \Big\} / \Big[f_z^2 \big(f_x^2 + f_y^2 + f_z^2\big)^2 \Big]$$

where f(x,y,z) is the function describing the shape of LCPs. The distribution of the function K on the real surface of LCPs f(x,y,z) = h showed that the areas of minimum values of the function K form channels through which the lateral diffusion of membrane proteins is easier than in the neighborhood.

These results help to visualize processes of lateral diffusion of membrane proteins inside LCPs, thus, being a basis for quantitative modelling of protein crystal growth during *in meso* crystallization experiments.

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SAS studies of apoferritin-based particles against COVID-19

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COVID-19 pandemic poses severe threats for humanity. Development of vaccines and drugs against SARS-CoV-2 is of the prior necessity nowadays and in the nearest future [1]. One of the promising solutions is the development of vaccines against coronaviruses is a vaccine based on self-assembling nanoparticles from chimeric structures of viral S-protein and apoferritin. These assembled constructs represent the protein coat of apoferritin with S-protein trimers. The similar approach was shown very efficient for influenza viruses [2] and might be efficient for COVID-19.

In this work we designed chimeric recombinant proteins consisting of apoferritin subunit and a part of the S-protein of SARS-CoV-2. These proteins were expressed and purified from *E.coli* cells and the assembly of the particles was checked by small-angle scattering method on the instrument Rigaku, MIPT, Dolgoprudny, Russia. The data showed the partial assembly of the particles and further construction modifications are needed to improve the self-assembly of the whole complex. The reasons that can affect the assembly and stability of the particles are discussed.

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Voltammetric study of the contact properties of hydrated multi-dimensional YSZ nanoparticles

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Adsorption and high surface curvature of nanoparticles significantly affect their electronic structure and can lead to new important effects of low-dimensional state [1]. The dimensional effects that occur at the contact of hydrated nanopowder YSZ - systems are extremely interesting due to their possible application [2].

In this work, the contact parameters of hydrated (85% humidity) Yttrium-Stabilized Zirconium oxide (YSZ) nanoparticles with the same chemical composition, but different size (7.5 and 10nm) were studied by voltammetry (see Table. 1). The nonlinear nature of the dependence of their electrical properties on direct current is established: the diode volt-ampere characteristic (V-I characteristic, Fig.1) is obtained, and the limiting electrical parameters are studied (Table 1). The effect can be extremely important for the development of semiconductor electronic systems from chemically homogeneous materials.

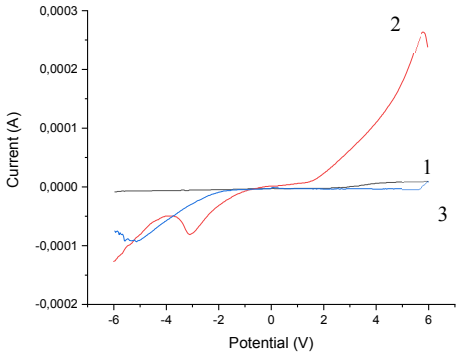

Fig.1. The group of VAC heterojunctions obtained at 85% humidity at the contacts of samples of the composition ZrO_2 – 0 mol% Y_2O_3,(1), ZrO_2 – 3 mol% Y_2O_3 (2) and ZrO_2 – 8 mol% Y_2O_3 (3).

Table 1

Limit electrical parameters of structures depending on the percentage of Y2O3 content.

Composition / Operating parameter	0 mol% Y2O3	3 mol% Y2O3	8 mol% Y2O3
Peak reverse voltage, V	-1,8±0,1	-2,5±0,1	-2±0,1
Peak reverse current, μA	5±5	70±10	100±10
Peak forward voltage, V	6±0,5	>6	6±0,5
Peak forward current, μA	5±5	250	5±5

The study was performed in the scope of the H2020/MSCA/RISE/SSHARE number 871284 and the RO-JINR Projects within the framework of themes FLNP JINR: 04-4-1105-2011/2022 and 03-4-1128-2017/2022.

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The RBS study of thin-films copper oxide on the substrate glass/ITO

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P-type oxide semiconductors based on copper oxide (I) and (II) (Cu_2O and CuO) are widely used in modern technologies of photo- and optoelectronics as photoelectric converters (PECs), photo-diodes, optoelectronic displays, etc. Both semiconductors have a high optical transmittance in the visible and near infrared (the band gap varies from 2 to 2.2 eV for Cu_2O [1, 2] and from 1.2 to 1.9 eV for CuO [1, 3]).

Optically transparent thin CuO films with p-type conductivity were deposited on pre-cleaned glass substrates coated with ITO (indium tin oxide film) by the SILAR method (Fig. 1) at n. at. in a ratio of 1: 3,3 ($CuSO_4 \times 5H_2O + Na_2S_2O_3$).

The optical absorption spectra of thin-film structures show a pronounced absorption edge in the region of 320 - 700 nm for CuO, which agrees with the known works [4]. The calculated (according to the Planck formula) band gap Eg was 1.64 to 1.98 eV.

It was found that with a decrease in the thickness of the p-CuO films, the absorption value decreases, which is important for practical application.

The RBS method was used to determine the distribution profile of the layer's composition. The measurements were carried out on the EG-5 accelerators (JINR, FLNP). The studies were carried out at the angle of incidence beam of He^+ ions (2.0 MeV) $\alpha = 30^o$ and 60^o and the scattering angle $\theta = 170^o$. The energy spectrum was obtained (Fig. 1). The spectra were processed using the standard SIMNRA 7.02 program.

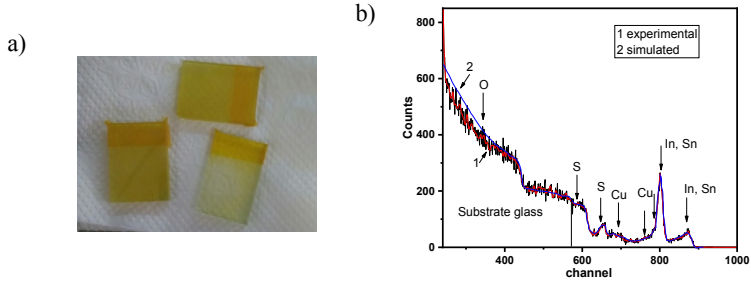

Fig. 1. p-CuO films obtained by the SILAR method (a); experimental RBS spectrum of ^{4}He + (2.0 MeV) helium ions of a CuO thin film on a glass / ITO substrate (b).

It was found (Fig. 1b) that the first layer (CuO) has a relatively small thickness and a high degree of inhomogeneity. The first and subsequent atomic layers contain insignificant concentrations of heavy elements In and Sn. related to the second layer of the ITO semiconductor film ((In□O□) 0.9 - (SnO□) 0.1).

A residual component of the chemical precursor sulfur (S), which can affect the physical properties of the structure, was detected by high-precision RBS modeling in the composition of the CuO thin-film structure. The issue requires additional study.

The study was performed in the scope of the Poland- JINR and RO-JINR Projects within the framework of themes FLNP JINR 03-4-1128-2017/2022.

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