CMRNS

Workshop on Condensed Matter Research by Means of Neutron Scattering Methods

4–7 July 2015, Constanta, Romania

Book of Abstracts

Joint Institute for Nuclear Research

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Organized by

Ovidius University of Constanta, Constanta, Romania
and
Joint Institute for Nuclear Research, Dubna, Russia

Sponsored by

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CMRNS is dedicated to the centenary of the birth of Fyodor L. Shapiro

(1915 – 1973)

Contents

Poster Session

Preface

On behalf of the International Advisory Committee and Local Organizing Committees, we welcome you to the **WORKSHOP on Condensed matter research by means of neutron scattering methods (CMRNS-Dubna).**

CMRNS-Dubna is a joint event of the 15th International Balkan Workshop on Applied Physics and Materials Science.

CMRNS-Dubna is hosted by Ovidius University of Constanta, and supported by the Balkan Physical Union, the Romanian Physical Society, Romanian Academy, Academy of Romanian Scientists, Joint Institute for Nuclear Research, Dubna.

The CMRNS topics will highlight results of interdisciplinary research and development of neutron instruments and techniques at IBR-2 reactor.

CONFERENCE TOPICS:

1. Condensed Matter Physics
2. Materials Science
3. Soft Matter (biological nanosystems, lipid membranes, polymers, magnetic elastomers, ferrofluids)
4. Life and Earth Sciences

CMRNS is dedicated to the centenary of the birth of **Fyodor L. Shapiro** (1915 – 1973), an outstanding Soviet physicist, who provided fundamental contribution to establishment and development of the experimental facilities and basic research areas at the Frank Laboratory of Neutron Physics (http://flnp.jinr.ru/25/), Joint Institute for Nuclear Research (http://www.jinr.ru/).

The main objective of **CMRNS-Dubna** is to offer overviews of several important research issues in the field and to provide opportunities for cooperation developments.

Organizing Committee

CMRNS 2015 PROGRAM

DATE	TIME	ACTIVITY
4 July	15.30 – 16.30	Registration
	16.30 – 18.00	Welcome party

DATE	TIME	ACTIVITY
5 July	9.30 – 10.00	Registration
	10.00-10.15	Opening ceremony
	10.15-10.45	Emil Burzo
	10.45-11.15	Yulia Gorshkova
	11.15-11.45	Sergey Kichanov
	11.45-12.00	Coffee Break
	12.00- 12.30	Gizo Bokuchava
	12.30 - 13.00	Tatiana Ivankina
	13.00 - 13.30	Oleksandr Ivankov
	13.30 - 14.30	LUNCH

	14.30 - 15.00	Andrey Rogachev
	15.00 - 15.30	Maria Balasoiu
	15.30 - 16.00	Coffee break
	16.00 - 17.00	Victor Ciupina
	17.00-17.30	Tetiana Popiuk
	18.30 – 20.30	BANQUET

DATE	TIME	ACTIVITY
6 July	10.00-10.30	Dmitry Nikolaev
	10.30-11.00	Tatiana Lychagina
	11.00-11.30	Coffee Break
	11.30-12.00	Anatolii Nagornyi
	12.00-12.30	Ihor Hapon
	12.30-14.00	LUNCH
	14.00-16.00	Round Table

DATE	TIME	ACTIVITY
7 July	10.00 -12.00	Poster Session
	12.00 - 12.30	Closing ceremony
	12.30 – 14.00	LUNCH

Invited Lectures

Pressure effects on the magnetic behaviour of rare-earth-cobalt compounds

Burzo E.

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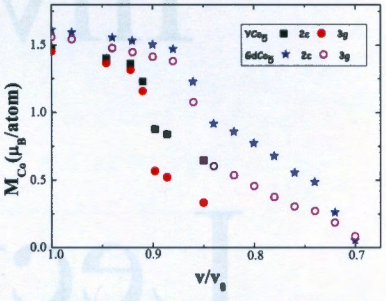
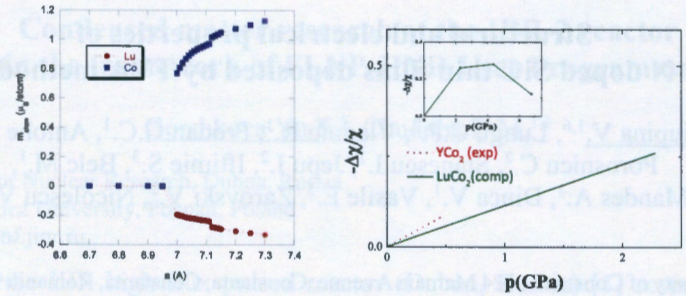
The effects of volume variations, simulating pressure effects, on the magnetic properties of RCo_5, R-Co-B or RCo_2 with R = Y or Lu, Gd compounds are analysed by using band structure calculations. The response of pressure, volume variations, respectively is dependent on the localization degree of cobalt moment. When cobalt has a high degree of localization as in RCo_5 (R = Y, Gd) compounds, there is a transition from high spin state to low spin one, at a reduced volume $v/v_0 = 0.90$ (R = Y) or 0.85 (R = Gd). At the transition, there is a higher decrease of M_{Co} at 3g sites than at 2c ones. Then, a linear decrease of cobalt moments, can be shown, being nil at $v/v_0 = 0.7$ – Fig.1.



For YCo_4B, there is a direct collapse of cobalt moment at 6i site, while at 2c ones, a transition from high spin to low spin site is observed. The above behavior can be correlated with the values of magnetic moments at normal conditions, higher by $\cong 1$ μ_B at Co (2c) site.

The behavior of $LuCo_2$ exchange enhanced paramagnet, as effect of pressure, volume variation is also analysed. The magnetic susceptibility decreases with pressure up to 2.3 GPa, then is nearly constant and finally decreasing as effect of pressure – Fig.2. For $p < 2.3$ GPa, a value $d\log\chi/d\log v = -12.2$ was obtained. This is close to that experimentally determined at $p \leq 0.45$ GPa, for YCo_2, of -14 ± 2.



The evolution with pressure of the cobalt magnetic behavior, in the above compounds are analysed in correlation with changes in their band structures.

This work was supported by the Romanian Ministry of Education and Research (UEFISCDI), grant no. PN-II-ID-PCE-2012-4-0028.

Structural and electrical properties of N doped SiC thin films deposited by TVA method

Ciupina V.[1,6], Lungu C.P.[2], Vladoiu R.[1], Prodan G.C.[1], Antohe S.[3], Porosnicu C.[2], Stanescu I.[1], Jepu I.[2], Iftimie S.[3], Belc M.[1], Mandes A.[1], Dinca V.[1], Vasile E.[5], Zarovski V.[2], Nicolescu V.[4]

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Ionized nitrogen doped Si-C thin films at 200°C substrate temperature were obtained by Thermionic Vacuum Arc (TVA) method. To increase the energy of N, C and Si ions, -400V, -600V and -1000V negative bias voltages was applied on the substrate. The 200nm thickness carbon thin films was deposed on Si and glass substrate and then 400nm, 600nm and 1000nm N-SiC coatings on carbon thin films was deposed. To characterize the structure of as-prepared N-SiC coatings, Transmission Electron Microscopy (TEM), High Resolution Transmission Electron Microscopy (HRTEM) and X-Ray and Photoelectron Spectroscopy (XPS) techniques was performed. The crystallinity of N-SiC thin films increase with increasing of acceleration potential drop, i. e. with energy of N, C and Si ions.

Electrical conductivity was measured comparing the potential drop on the structure with the potential drop on a series standard resistance in a constant current mode. Significant increases in the acceleration potential drop lead to a variation of crystallinity and electrical conductivity of N-SiC coatings.

Keywords: SiC nanostructures, TVA method, TEM, HRTEM, XPS, electrical conductivity.

Acknowledgments

This work was supported by the JINR-Romania Scientific Project No. 34/23.01.2015 item 48.

Condensed matter research at the IBR-2 reactor in the framework of FLNP JINR User Programme

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In 2012, the IBR high flux pulsed reactor (Dubna, Russia) [1] resumed its regular operation at a nominal power for scientific research. Neutron scattering investigations at IBR-2 reactor cover an extensive field of research in condensed matter physics, materials science, chemistry, biophysical, geophysical and engineering sciences (Fig.1).

The IBR-2 reactor is operated according to the User Policy Programme[2]. Calls for proposals are issued twice a year. The proposals are peer-reviewed and rated. The beam time for experiments is allocated on the basis of the reviews by Expert Committees. At present, about 200 experiments are performed annually by scientists from more than 20 countries (Fig.1) at IBR-2 instruments in the framework of the User Programme.

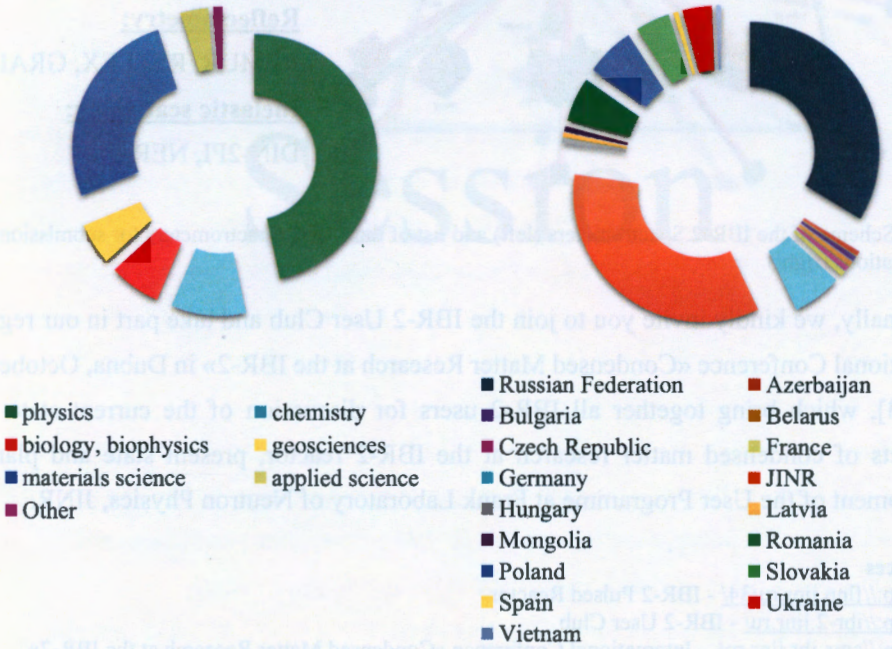
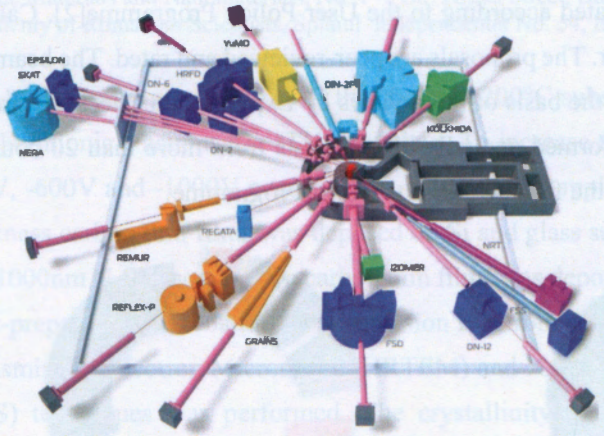


Fig.1. Distribution of proposals by science (left) and by applicant's affiliation (right) in 2014. Data are adopted from IBR-2 User Club site [2].

Currently, the spectrometer complex of the IBR-2 pulsed reactor consists of 12 instruments available for scientific research: 6 diffractometers, 1 small angle neutron scattering spectrometer, 3 reflectometers and 2 inelastic neutron scattering spectrometers (Fig.2). There are also 3 new facilities under construction: diffractometer for studying microsamples (DN-6), neutron imaging instrument for radiography and tomography studies (NRT) and Fourier spectrometer for stress measurements (FSS). Additionally, a significant number of proposals (about 30% of the total number of submitted applications) for the YuMO spectrometer has led to the discussion of a new project «High-flux small-angle neutron scattering spectrometer (SANS-S)».



Diffraction:
HRFD, DN-2, DN-12,
SKAT-EPSILON, FSD
Small-angle scattering:
YuMO
Reflectometry:
REMUR, REFLEX, GRAINS
Inelastic scattering:
DIN-2PI, NERA

Fig.2 Scheme of the IBR-2 Spectrometers (left) and list of the IBR-2 Spectrometers for submission of applications (right)

Finally, we kindly invite you to join the IBR-2 User Club and take part in our regular International Conference «Condensed Matter Research at the IBR-2» in Dubna, October 11 – 15 [3], which bring together all IBR-2 users for discussion of the current state and prospects of condensed matter research at the IBR-2 reactor, present state and plan of development of the User Programme at Frank Laboratory of Neutron Physics, JINR.

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[2] http://ibr-2.jinr.ru/ - IBR-2 User Club
[3] http://cmr-ibr.jinr.ru/ - International Conference «Condensed Matter Research at the IBR-2»

Oral Session

Small angle neutron scattering investigations of magnetic elastomers polymerized in transversal and longitudinal magnetic fields

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Magnetic and magnetorheological elastomers (MEs and MREs) are composite materials prepared from an elastic matrix into which magnetizable nano or micro particles are dispersed. Similar to the case of magnetic fluids and magnetorheological suspensions in magnetic field, the magnetic phase tends to form aggregates, determining considerably changes in the physical characteristics of MREs.

Fig.1. Magnetorheological elastomer: shape and size.

The synthesis and the study of structure and physical properties of MEs and MREs, materials combining the functional properties of elastic polymers and nanomagnetic/micro particles, are considered as a perspective way to provide the understanding of construction principles of a wide class of materials for electronics, electrical engineering, medicine, aero- and cosmic industries [1-3]. Also from the fundamental point of view it is needed a comprehensive analysis of the relationship between the macroscopic and microscopic properties of the dispersed magnetic phase structures behaviors [4,5].

In the present paper results of the small angle neutron scattering investigation of the structure of ferroelastomers composed of polydimetylsiloxane with Fe_3O_4 ferrofluid embedded before the polymerization process [6,7,8] are presented and discussed.

Acknowledgements The authors acknowledge the financial support through the grant of the Romanian Governmental Representative at JINR No.32 /23.01.2015 item 16.

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Neutron diffraction potentialities for residual stress studies at the IBR-2 pulsed reactor

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The investigation of internal mechanical stresses in materials is of fundamental as well as of applied importance. The neutron diffraction technique for stress investigations came into use in the mid 1980s and since then it has become widely applied due to a number of significant advantages over conventional methods. The most important advantage is that neutrons can penetrate matter to a depth of 2-3 cm in steels and up to 10 cm in aluminium. The advantages of neutron diffraction are so overwhelming that in recent years diffractometers for internal stress investigations have been built almost in all advanced neutron centres in the world.

The greater part of the studies is concerned with the determination of residual stresses in industrial products and structures. The most frequent source of stresses is various technological processes. These studies are of interest for manufacturers from the viewpoint of creating optimum properties of materials and optimization of technological production processes. The results of these studies help to create optimum residual stress states in different cross sections of the component part and consequently, improve its performance characteristics and service life.

Another important direction of research activity is investigations of residual stresses and mechanical properties of advanced materials, such as composites or gradient materials as well as different steel grades. Within the framework of these investigations, the coexistence of different phases in one material and their joint impact on the elastic properties and residual stresses in the material are studied. These investigations are important for the creation of materials with physical-chemical and elastic properties specified in advance. The results of these studies make it possible to create new materials with predictable properties and behaviour

At present, JINR is the only scientific centre in Russia where regular world-class neutron diffraction investigations of residual stresses are conducted. For this purpose, the Fourier stress diffractometer (FSD) has been constructed at the IBR-2 high-flux pulsed reactor (Fig. 1). The FSD is using reverse time of flight (RTOF) method in combination

with the fast Fourier chopper for neutron beam intensity modulation. The FSD design satisfies the requirements of high luminosity, high resolution and specific sample environment. The collimator system guarantees a minimum gauge volume of 2x2x2 mm^3. For precise sample positioning with an accuracy of ~0.05 mm and better four-axis HUBER goniometer is used (the max. carrying capacity ~300 kg). A mechanical testing machine allows *in-situ* tension or compression experiments up to a load of 20 kN and sample temperatures up to 800°C.

In the paper, the status of FSD is reported and potentialities are demonstrated with several examples of investigations performed. The technical characteristics and description of FSD are given in [1, 2].

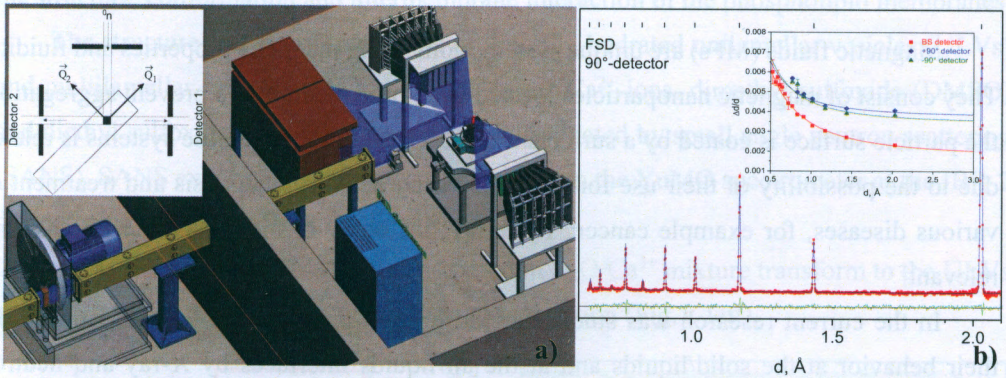

Fig. 1. **a)** 3D model of the Fourier stress diffractometer FSD at the IBR-2 reactor (FLNP JINR, Dubna). The basic functional units of the FSD are the long mirror neutron guide with variable diaphragms, the fast Fourier chopper, the detector system consisting of ±90°-detectors with radial collimators and a backscattering detector, HUBER goniometer at the sample position, auxiliary equipment (furnaces, testing machines, etc.), specialised data acquisition electronics including RTOF analysers. **Inset:** The scheme of the experiment for residual stress studies in a bulk object. Incident and scattered (at angles $2\theta = \pm 90°$) neutron beams are formed by diaphragms or radial collimators defining a gauge volume within the sample. Measurement of neutron diffraction patterns by ±90°-detectors allows simultaneous determination of strains in two mutually perpendicular directions. **b)** A part of the neutron diffraction pattern measured from an α-Fe standard sample using the 90° detector. Shown are the measured data points as well as results from a Rietveld full profile analysis giving the theoretical model pattern through the data points and the difference curve. **Inset:** resolution function for FSD detectors.

This work was partially supported by the Romania-JINR Programme 2014-2015, by the Russian Foundation for Basic Research (project 15-08-06418_a) and jointly by RFBR and the Moscow Region Government (project 14-42-03585_r_center_a).

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Reflectrometry studies of the structure and stability of ferrofluids at the solid-liquid and air-liquid interfaces

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Magnetic fluids (MFs) are unique systems combining magnetic properties and fluidity. They consist of magnetic nanoparticles located in a liquid medium. To prevent aggregation, the particle surface is coated by a surfactant layer. Great interest in these systems is related due to the possibility of their use for controlled drug delivery, diagnosis and treatment of various diseases, for example cancer. Therefore, the study of biocompatible FF are very relevant.

In the current research was studied the adsorption properties of biocompatible MFs their behavior at the solid/liquids and at the air/liquids interfaces by X-ray and neutron reflectometry. It was shown the effect of gravity to the destabilization of the magnetic fluid. The structural organization of the nanoparticles at the studied interfaces was discussing. Also, it was held comparative analysis of magnetic fluid prepared on a non-polar solvent and we observed a similar structure.

Keywords: neutron reflectometry, x-ray reflectometry, adsorption of magnetic particles, magnetic fluids.

Structure and phase transitions of lipid membranes in the presence of ions and polar molecules: Small angle neutron scattering investigation

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Lipid membranes are the basic building blocks for almost all living organisms. Cell membranes consist of the phospholipid bilayer with embedded proteins. The cell membrane is selectively permeable to ions and organic molecules and controls the movement of substances in and out of cells. On the other hand the ions and polar molecules also affect on the structure, conformation and intermembrane interaction of the phospholipid membranes.

The structure and phase transitions of the fully hydrated unilamellar vesicles (ULVs) and multilamellar vesicles (MLVs) DMPC in the Ca^{2+} ions, dimethyl sulfoxide (DMSO) and diethyl sulfoxide (DESO) presence was investigated by small angle neutron scattering (SANS). SANS experiments have been performed on the YuMO spectrometer at the IBR-2 pulsed reactor in FLNP JINR (Dubna, Russia).

It was shown that MLVs DMPC prepared in D_2O/Ca^{2+} mixture transform to the ULVs spontaneously with increasing of the Ca^{2+} concentration (Fig.1, left).

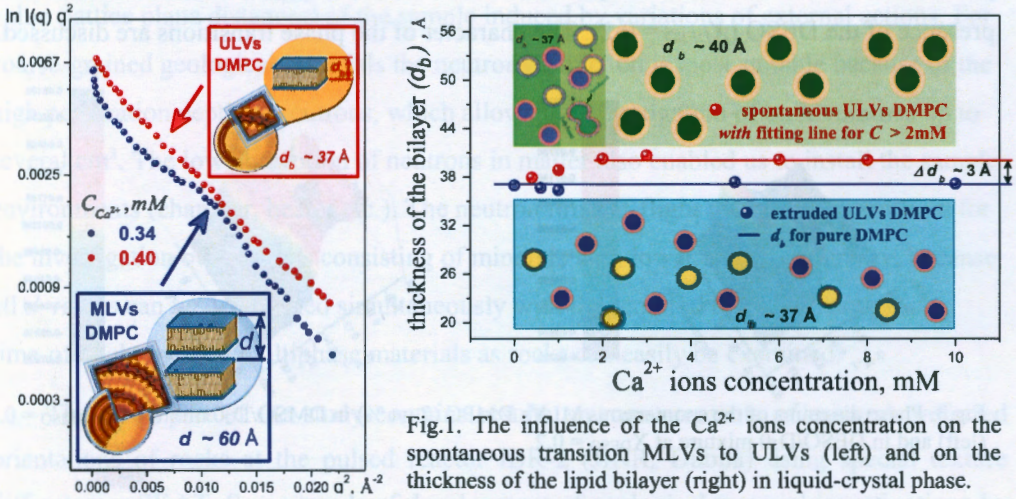

Fig.1. The influence of the Ca^{2+} ions concentration on the spontaneous transition MLVs to ULVs (left) and on the thickness of the lipid bilayer (right) in liquid-crystal phase.

Fusion of the ULVs DMPC in the presence of the divalent cations Ca^{2+} (Fig.1, right) and sulfoxides (Fig.2) was observed. It turned out that the ULVs fusion is caused by two factors: time and increasing of the DMSO and DESO concentration. The present work confirms the hypothesis about a crucial role of the hydrophobic interactions in the intermembrane

interaction in the presence of sulfoxides. However, it should be noted that these hydrophobic interactions are stronger in the presence of DESO. At first, DESO causes the fusion of the ULVs about 1/2 hour after samples preparation, while this process occurs in an hour in the presence of DMSO. At the second, the investigation in short-term time scale shown that formation of the MLVs take place at $X_{DESO} = 0.3$ and $X_{DMSO} = 0.4$.

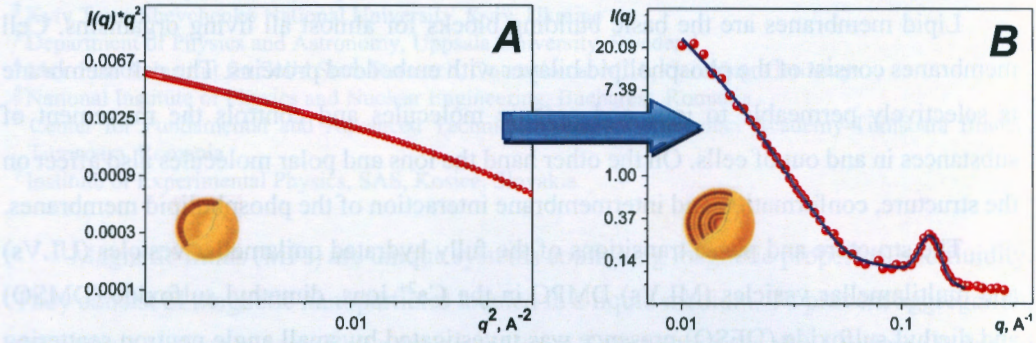

Fig.2. SANS curves on ULVs DMPC (2 wt %) in DMSO/D_20 mixture at $X_{DMSO} = 0.2$ in liquid-crystalline phase at T = 55 °C after preparation (A) and 1 hour later (B).

The phase transitions of the spontaneous MLVs DMPC in the DMSO and DESO presence was investigated in wide temperature range (Fig.3). The temperatures of the main phase transition are 35.2°C at the presence of the DMSO ($X_{DMSO} = 0.2$) and 33.6°C at the presence of the DESO ($X_{DESO} = 0.2$). The character of the phase transitions are discussed.

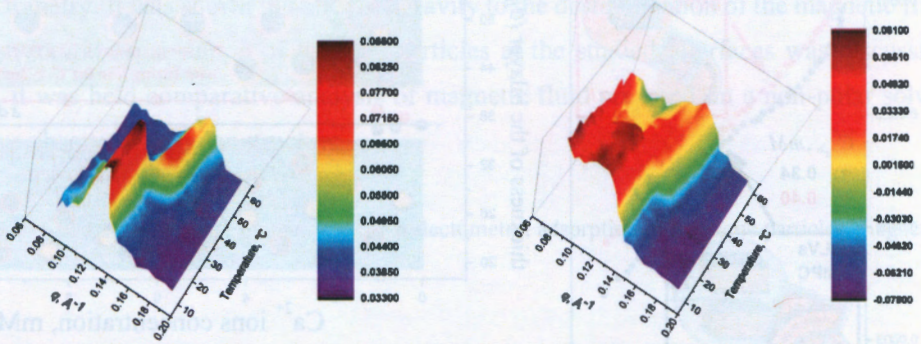

Fig.3. Phase diagrams of the spontaneous MLVs DMPC (2 wt %) in DMSO/D_20 mixture at $X_{DMSO} = 0.2$ (left) and in DESO/D_20 mixture at $X_{DESO} = 0.2$.

This work was supported by the Romania – JINR (Dubna) Programme 2014 – 2015.

Why do geoscientists use neutron diffraction?

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The principle advantages of neutron diffraction based on phenomenal properties of neutron which permit to extend an aspect range of solid-state physics, geology and geophysics are analyzed:

- determination of the structure of rock-forming minerals,
- texture measurement and study of texture formation processes in rocks,
- investigation of the kinetics of phase transitions in connection with the origin of the seismic anisotropy and geodynamic problems, and
- study of residual and local strains/stresses of rock.

Crystallographic mineral preferred orientations (textures) are one of the important fabric elements of rocks, which give us the unique information on the mechanisms of evolution of Earth's lithosphere. Neutron diffraction has some advantages especially for geological materials. Neutron diffraction provides experimental data on changes of *d*-value (lattice plane distances) of the sample induced by variations of external actions. For coarse-grained geological materials the neutron diffraction is most suitable because of the high penetration depth of neutrons, which allows the investigation of bulk volumes up to several cm^3. The low absorption of neutrons in matter also enabled us to install the sample environments (chamber, heater etc.). The neutron time-of-flight method is appropriate for the investigation of materials consisting of minerals with lower crystal symmetry, because all *d*-values can be determined simultaneously with the required high precision. Using time-of-flight method multiphase materials as rocks can easily be examined.

The basic part of the study contains results on measurements of mineral preferred orientations of rocks at the pulsed reactor IBR-2 (JINR, Dubna) using special texture diffractomer SKAT. Some trends of development of geological material investigations by means of neutron diffraction for the purpose of fundamental Earth sciences are discussed.

Small angle neutron scattering spectrometer YuMO for soft matter investigations

Ivankov O.I.[1,2,3], Soloviov D.V.[1,2,3], Rogachev A.V.[1,2], Kovalev Yu.S.[1,2], Sirotin A.P.[1], Petukhova T.B.[1], Kirilov A.S.[1], Soloviev A.G.[1], Solovieva T.M.[1], Gordeliy V.I.[1,2,4,5], Kuklin A.I.[1,2]

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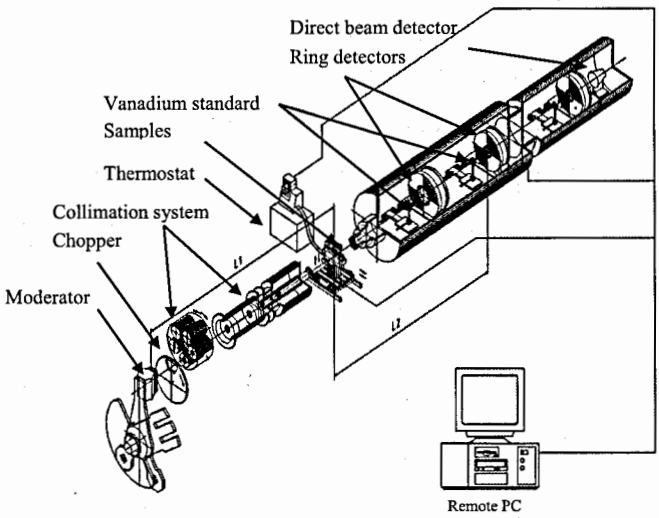

Fig 1. Scheme of the YuMO spectrometer with two-detector system.

The possibilities of the modernized spectrometer YuMO at high flux IBR-2 pulsed reactor due to automation of separate units are shown [1]. Main unique devices due to modernization are presented [2, 3]. The wide q-range, absolute scale and dynamic q-range was shown [4]. Standard configuration of the spectrometer include thermobox connected with liquid thermostate are presented. Advantages of the upgraded spectrometer are shown. The main applications of spectrometer are presented.

Table 1. Main parameters of the YuMO spectrometer

Parameters	Value
Flux on the sample (thermal neutrons)	$10^7 - 4x10^7$ n/(s cm^2)
Used wavelength	0.5 Å to 8 Å
Q-range	$7x10^{-3} - 0.5$ Å^{-1}
Dynamic Q-range	q_{max}/q_{min} up to 100
Specific features	Two detectors system, central hole detectors
Size range of object	500 – 10 Å
Intensity (absolute units -minimal levels)	0.01 cm^{-1}
Calibration standard	Vanadium during the experiment
Size of beam on the sample	8 – 22 mm^2
Collimation system	Axial
Detectors	He^3 -fulfiled, home made preparation, 8 independent wires
Detector (direct beam)	^{6}Li-convertor (home made preparation)
Condition of sample	In special box in air
Q-resolution	low, 5-20%
Temperature range	-20°C -+150°C
Number of computer controlled samples	25
Background level	0.03 – 0.2 cm^{-1}
Mean time of measurements for one sample	1 h
Frequency of pulse repetition	5 Hz
The instrument control software complex	**SONIX** [5]
Controlling parameters	Starts (time of experiments), power, vandium standard position, samples position, samples box temperature, vacuum in detectors tube.
Data treatment	SAS, Fitter [6-7]

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The optical properties forming in optical-active materials: neutrons studies

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My talk is focused on resent experimental results of studies of optical materials by means of neutron diffraction and small angle scattering technics at IBR-2 high flux pulsed reactor in Dubna, Russia.

At present, the urgent problem of structural chemistry and materials science is to produce optical materials with the possibility of varying their optical properties at the stage of synthesis. In this regard, the application of colloidal chemical methods is most promising for solving this problem, making it possible to obtain materials characterized by high homogeneity of the distribution of optically active ions more easily introduced into the crystal matrix, and most importantly, the possibility of forming complex composite systems with a controllable redistribution of activator ions between the components.

The most promising and widely studied materials for laser and photoluminescence equipment are crystalline phosphors based on yttrium aluminum $Y_3Al_5O_{12}$ (YAG) and lutetium aluminum $Lu_3Al_5O_{12}$ (LuAG) garnets. In our experiment, neutron diffraction spectra have been obtained for composite phosphors $Y_3Al_5O_{12}:Ce^{3+}/Lu_2O_3$ and $Lu_3Al_5O_{12}:Ce^{3+}/Lu_2O_3$ for different concentrations of Lu_2O_3. The modification of luminescent properties by Lu_2O_3 doping in $Lu_3Al_5O_{12}:Ce^{3+}+Lu_2O_3$ is drastically different is comparison with $Y_3Al_5O_{12}:Ce^{3+}+Lu_2O_3$. The difference in the effects of the introduction of Lu_2O_3 for phosphors $Lu_3Al_5O_{12}:Ce^{3+}/Lu_2O_3$ and $Y_3Al_5O_{12}:Ce^{3+}/Lu_2O_3$ on the formation of their optical properties can be explained by the processes of diffusion of cerium ions from the $Lu_3Al_5O_{12}:Ce^{3+}$ matrix to Lu_2O_3, which is accompanied by a decrease in their concentration in $LuAG:Ce^{3+}$. When introducing Lu_2O_3 into $Y_3Al_5O_{12}:Ce^{3+}$ there also occurs a redistribution of Ce^{3+} ions in the system, but it takes place not between the phase $Y_3Al_5O_{12}:Ce^{3+}$ and Lu_2O_3, but between additional phases being formed of $Y_{3-x}Lu_xAl_5O_{12}$ and/or $Lu_3Al_5O_{12}$, in which Ce^{3+} ion luminesces well.

The promising materials for optical filters are silicate glasses doped by transition and rare-earth metal oxides. These glasses doped by cerium and titanium oxides have selective light absorption and characterized by high thermal stability and ultra-violet radiation protection. It was assumed, that unique physical properties of these glasses can be result of a complex oxide nanoparticles Ce-Ti-O forming. In the present work most attention is focused on the research of structure aspects of optical properties formation in silicate glasses with different initial oxides TiO_2/CeO_2 molar concentration by means of small angle neutron scattering.

The formation of complex oxide Ti-Ce-O nanoparticles in the silicate glasses was revealed. At fixed cerium oxide molar concentration $x(CeO_2)=2.0$ the variation of TiO_2 relative concentration in low molar concentration range 0.3-1.0 is reason the average size of formed nanoparticles increases with $dR_g/dx \approx 4.3(1)$, but at high titanium oxide concentration $x(TiO_2) > 1.0$ this coefficient approximately twofold decreased to 2.2(1). This fact can be explained by a model with two different types of nanoparticles formed in the silicate glasses. So at small molar concentrations ratio of initial CeO_2/TiO_2 oxides the nanoparticles are formed by predominately from oxygen, trivalent cerium Ce^{3+} and tetravalent titanium ions Ti^{4+}. With relative concentration CeO_2/TiO_2 increasing a valence state of cerium ions changes to tetravalence Ce^{4+} and this fact are reason formation of another nanoparticles type, which characterized by larger average size and another mechanism of optical properties forming.

The work has been supported by the RFBR and the Ministry of Investment and Innovation of Moscow region under grant № 14-42-03641_r_centr_a.

Neutron diffraction investigation of rail wheel steel texture

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Study of the factors controlling the structure and properties of rail wheel steel is a very important task because it allows optimizing of steel composition and temperature regimes for mechanical properties improvement. The production technology of the rail wheels includes such operations as forging, press forming and rolling that can result in texture formation. The subsequent temperature treatment (annealing, quenching and tempering for rim) can also influence texture changing. Besides, texture formed as a result of railway wheel usage influences on their strength and operating life. Neutron diffraction is a powerful nondestructive tool for global texture investigation in the volume of the material.

In this work the crystallographic texture for a set of wheel steel samples with different regimes of thermo-mechanical treatment and with and without doping by systemAl-Mg-Si-Fe-C-Ca-Ti-Ce has been measured by neutron diffraction. The texture measurements have been carried out by neutron diffraction using time-of-flight technique at SKAT diffractometer [1-2] situated at IBR-2 reactor (Dubna, Russia). The three complete pole figures (110), (200), (211) of α-Fe phase in 5°×5°grid have been extracted from a set of 1368 spectra measured for each sample (Fig.1).

We had for texture investigation four samples from the wheel rim and four samples from the transitional zone between the wheel hub and disk. Namely in this transitional zone cracks sometimes appear under fatigue cycling tests. The samples 1 and 3 were cut from the modified steel wheel, whereas the samples 2 and 4 were cut from the conventional steel wheel. The samples 3 and 4 were undergone deformation according to technological operations of rail wheels production, and the samples 1 and 2 were undergone temperature treatment following this deformation. The samples volume was about $10cm^3$. So we had good grain statistics because the grain size in the both types of steel is about 25μm.

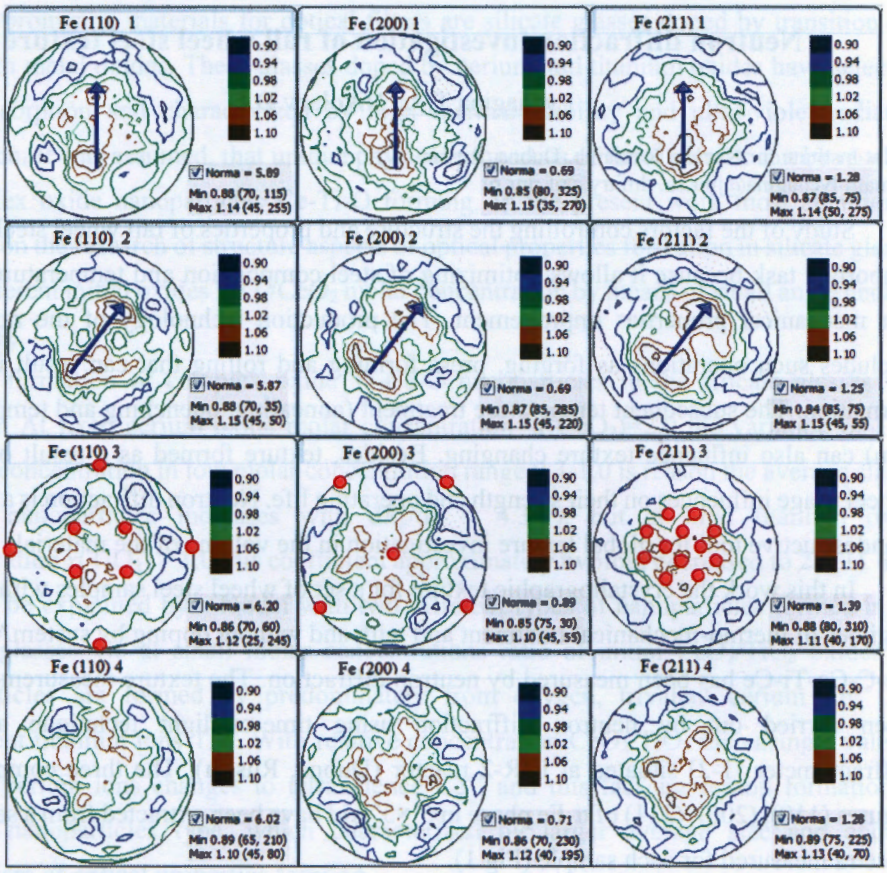

Fig.1. The smoothed pole figures (110), (200), (211) of α-Fe phase for four samples from the rail wheel rims. The red points mark the deformation texture component. The blue arrows demonstrate the texture component rotation in the sample 1 (from the modified steel) according to the sample 2 (from the conventional steel). The top raw is for the sample 1; the next one is for the sample 2, etc.

The resolution of SKAT texture spectrometer is rather high $\Delta d/d = 5\times10^{-3}$ at d=2.5Å and $2\theta = 90^{\circ}$. This resolution allows to have non-overlapped diffraction peaks for α-Fe phase of the steel. In Fig.2 the spectrum obtained as sum over 1368 individual measured spectra is presented to demonstrate SKAT resolution. The measuring time was 22 hours. It was used the local peak fit procedure for the PFs extraction [3-4].

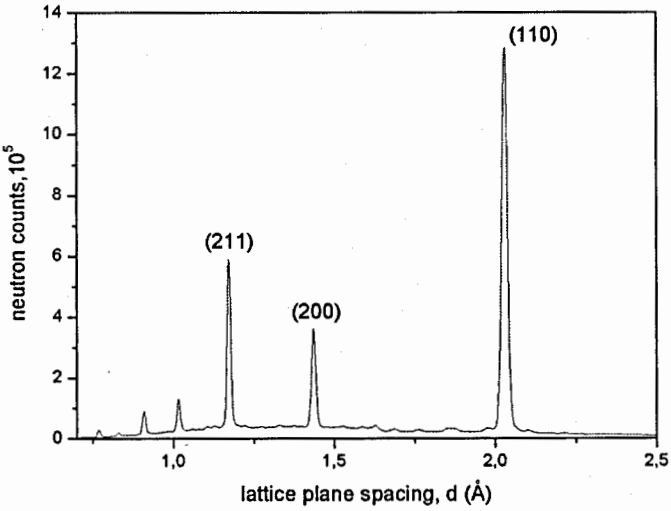

Fig. 2.The sum spectrum measured at SKAT for sample 1 from modified steel.

It was concluded that the steel modification and some changes in the heat treatment modes of the rail wheels from the experimental (modified) and the conventional (non-modified) steel lead to reorientation of texture component. The measurements at SKAT spectrometer were able to show properly the texture changes corresponding to the technological operations even in spite of the texture weakness in the investigated samples.

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Structure and stability of ferrofluids with surfactant excess by small-angle neutron scattering

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Colloidal suspensions of magnetic nanoparticles coated with surface-active agents (surfactants) to prevent an aggregation under various conditions are great of interest in condensed matter physics. They present an individual class of materials co-called as magnetic fluids (MF) or ferrofluids. Magnetic nanoparticles have a characteristic size of about 10 nm that corresponds to a single-domain state, thus determining a superparamagnetic behavior of the liquid system. This specific property of ferrofluids is very useful for different technological and biomedical applications [1-3].

In spite of relatively strong and hard-predicting interaction between magnetic nanoparticles MFs show a good stability as colloidal systems. Aggregation stability of ferrofluids is significantly determined by the interaction between molecules of surfactants in the solvent. The concentration of surfactant molecules in a solution is one of the important factors affecting on the stability of MFs, especially in the case when magnetic fluids contain some excess of stabilizer molecules. It is known in practice there is the optimal amount of surfactant in MFs at which ferrofluids have the most possible stability as colloidal liquid system. The present work was carried out within the framework of systematic investigations of the influence of surfactant excess on the structure of the different types MFs [4-8].

The small-angle neutron scattering (SANS) is one of the most informative scientific approach for structural studies of multicomponent nanosystems and particularly magnetic fluid [8]. The structural parameters of the classical magnetic fluids prepared on the base of decalin at different excess of oleic and myristic acids in MF's volume (up to 20 vol.%) were determined by SANS as well as the Guinier parameters for molecules of the above mentioned acids were eliminated by SANS. Additional comparison of oleic and myristic acids behavior dissolved in the decaline and dissolved in corresponding magnetic fluids

allows to evaluate the changing of interaction between the molecules of free (non-adsorbed) surfactant in the presence of magnetic nanoparticles. The structure parameters of polar ferrofluid stabilized by oleic and dodecyl-benzenesulfonic acids were obtained. In the case of polar MF the interparticle interaction in the system was considered by analyzing the effective structure factor.

Considered magnetic fluids are stable in respect of the formation of large aggregates of the magnetic nanoparticles in the studied range of the surfactant concentration. Comparison of the results with previously reported data for similar MFs based on benzene [4-6] is performed in the work.

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Neutron time-of-flight quantitative texture analysis

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The metallic alloys, as well as many natural or industrial materials, are nearly always polycrystalline materials. Therefore their physical or mechanical properties exhibit very often an anisotropy which is mainly due to the presence of preferred orientations or crystallographic texture described by an ODF (Orientation Distribution Function). Both aspects, characterizing the texture from one side and correlating it to the properties from the other side, are then essential in understanding and improving the metallic materials behavior.

An important step of texture analysis is pole figures processing and orientation distribution function (ODF) reconstruction [1-2]. The ODF could be reconstructed from the pole figures that are obtained from experimentally measured neutron time-of-flight diffraction spectra.

We present details of neutron time-of-flight diffraction spectra processing. The spectra were measured at SKAT [3-4] spectrometer shown in figure 1 at pulsed reactor IBR-2.

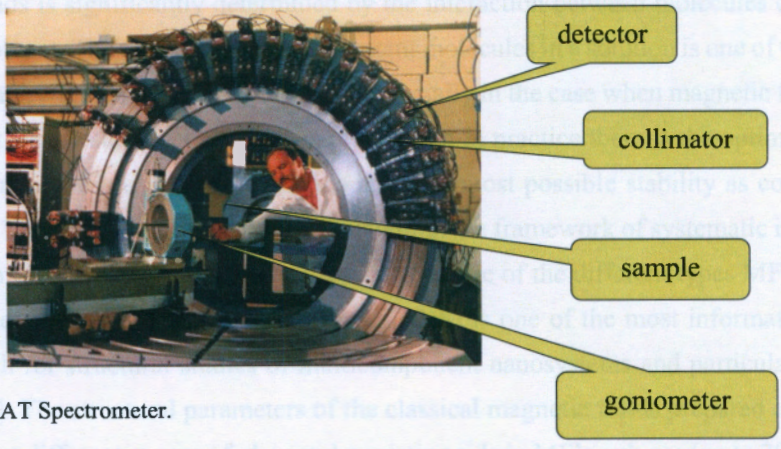

Fig 1 SKAT Spectrometer.

We also present examples of the quantitative texture analysis for the different metallic and non-metallic materials. Figure 2 illustrates the anisotropic behavior of the marble panels.

Fig. 2 Behavior of the marble panels on the economic building in Goettingen.

The experimental pole figures and strain pole figures for marble are presented below.

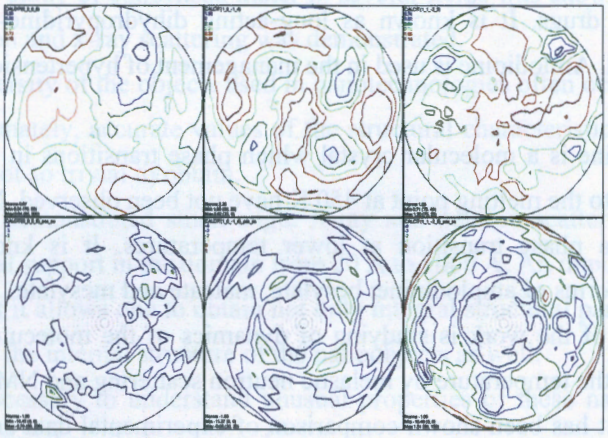

Fig. 3 Pole figures and strain pole figures of marble.

In the work the other examples of neutron texture analysis application are presented.

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Neutron scattering and NMR study of amlodipine besylate

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To product an electrical activity for reduction of cardiac and smooth muscle as well as conducting it in nervous cells requires of calcium ions. There are preparations that suppress excessive calcium entry into cells, promote relaxation of the walls of blood vessels and cardiac muscle and thus provide a free flow of blood. Amlodipine belongs to a new-generation of drugs. It is known as long-acting dihydropyridine-type calcium channel blockers [1, 2]. Amlodipine is used in the management of hypertension and coronary artery disease.

Amlodipine is a molecular crystal which phase transitions in the temperature range from 77 K up to the melting point at 450 K have not been observed. Nevertheless, it cannot be excluded a phase transition at lower temperatures. It is known that there are 3 polymorphic forms of amplodipine: besylate, maleate and mesylate.

The aim of the work is studying of dynamics of the molecule amlodipine besylate depending on the temperature by inelastic neutron scattering and NMR methods.

In work it has been shown comparison of experimental data and results obtained by "Monte-Carlo" method.

Acknowlegements:

Wasicki J., Pajzderska A., Bilski P. Faculty of Physics Adam Mickiewicz University Poznan, Poland

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Some possibilities of small-angle scattering techniques

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Small-angle scattering techniques is most performance method for investigation of different type of nano size systems.

Some examples study of condensed mater in several fields was shown. Comparisons of small-angle neutron and x-ray scattering was demonstrated.

High monodispersity of the objects used in nanotechnologies often occurs to be a key requirement. Unfortunately, accurate values of the structural characteristics of the objects with nano sizes are not so trivial to obtain.

As it has been demonstrated small-angle X-ray and neutron scattering gives us an excellent metrological support in the domain from 20 Å to 1000 Å. An important advantage of this method is that it allows one to obtain not only integral structural parameters but the important data about the internal structure of the nanoobjects as well.

The latter is necessary to understand unusual properties of these nanoparticles and develop new nanomaterials with the required properties.

Poster Session

Micropore formation in silicone rubber based membranes

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In this work, we present the fabrication method of microporous membranes based on silicone rubber and stearic acid, at various volume concentrations of the catalyst. We show that the dimensional distribution of the pores is significantly influenced by the catalyst concentration. We present the obtained results and discuss the influence of catalyst concentration on the pore distribution. The results give new insights into pore formation mechanisms in silicone rubber based membranes [1].

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Intermolecular interactions in ternary solutions of some pyridazium ylids described by the solvent empirical scales

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Pyridazinium ylids are zwitterionic compounds having separated charges on adjacent atoms from their molecules. The separated charges can be moved by the photons from the UV or VIS ranges. Ternary solutions can offer information about the interactions in which the pyridazimium ylids are involved in the two solvents used for binary solvent obtaining.

In the studies presented here, the zwitterionic compounds are spectrally active molecules and show a visible electronic absorption band which is sensible to the solvent. In binary solvents, water + ethanol and water + methanol, the wavenumbers in the maximum of the ICT electronic absorption bands of ylids increase with the water content increasing. The empirical scales of solvents can be used in order to describe the solvent influence on the electronic absorption spectra.

The wavenumbers in the maximum of the visible intermolecular charge transfer (ICT) absorption band recorded in ternary solutions of spectrally active molecules were correlated with the solvent empirical parameters $E_T(30)$, π^*, α, β.

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Nuclear and magnetic scattering components determination using nonpolarized neutrons

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Magnetic nanoparticles are one of the most interesting classes of material due to their numerous technical applications. Development and optimization of their obtaining process requires knowledge about their characterization, in particular, the size and particle size distribution measures.

The use of neutrons in magnetic materials characterization has the advantage of allowing to be obtained simultaneously the information on the physical and magnetic structure of the investigated system.

The effective cross section for the general scattering process relative to a scatterer nucleus according to [1] is defined as:

$$d\sigma / d\Omega = b^2 + 2bp\vec{q}\vec{\lambda} + p^2q^2 \qquad (1)$$

in which

b is the nuclear scattering length

p is the magnetic scattering length

λ is the versor of the incident to the sample neutron polarization direction;

$$\vec{q} = \vec{\varepsilon}\left(\vec{\varepsilon}.\vec{K}\right) - \vec{K}$$

where $\vec{q}$ is the vector of the magnetic interaction; $\vec{K}$ and $\vec{\varepsilon}$ are the the unit vectors of the magnetization direction of the sample, respectively of the orthogonal direction to the scattering plan (scattering unit vector).

Several methods of separate determination of nuclear and magnetic components of neutron scattering derived from relation (1) using polarized and unpolarized neutrons are known [2].

The present work describes the method of application the contrast variation technique [3, 4], for eliminating the need for the magnetic field application and the use of polarized

neutrons in the process to separate the nuclear and magnetic scattering from the colloidal disperse systems [5].

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On the modelling of the magnetic nanoparticles influence on elastomer matrix from SAS data

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[3] Computational Mathematics and Cybernetics Faculty, Moscow State University, Moscow, Russia
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Magnetic elastomers (ME's) represent a specific class of smart materials responding in a complicated way to the changes of external conditions. ME's are composed of magnetic nanoparticles and a low magnetic permeability polymer matrix. These composites are quite new, and the work on understanding their properties in dependence on the synthesis processes, composition, mechanical and magnetic fields, etc. is nowadays extensively progressing with regard to nano- or microtechnology.

These types of polymer nanocomposites are characterized by the coexistence of several different length scales: the average radius gyration of the polymer molecules (R_G), the average diameter of the nanoparticles (2r), and the average nearest-neighbor distance between the particles (d) [1].

A small angle X-ray scattering (SAXS) experiment on magnetic elastomers samples was performed on the Rigaku SAXS spectrometer at IMC, Prague, in the Q, momentum transfer value range of (0.004 - 1.1) A^{-1}.

The present work presents several modeling approaches for the mathematical description of the elastomer matrix behavior (Fig.1) in function of the particle concentration and magnetic field application during the preparation process. SAXS scattering curve of the elastomer matrix in log-log coordinates and best linear fits for 3 regions of Q, in the range (0.008-0.1) A^{-1} are given in Fig.1.

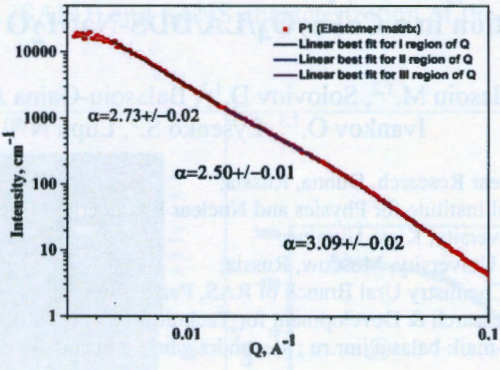

Fig.1 SAXS scattering curve of the elastomer matrix in log-log coordinates and best linear fits for 3 regions of Q, in the range (0.008-0.1) A^{-1}.

Acknowledgements The authors acknowledge the financial support from the Romanian Governmental Plenipotentiary Representative to JINR Grant No 32/23.01.2015 item 16.

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SANS investigation of particle concentration and temperature variation in a $CoFe_2O_4$/LA/DDS-Na/H_2O ferrofluid

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

Nowadays researches on developing ferrofluids with new types of particles, new synthesis methods, increased particle concentration, using different stabilization methods and compounds are in progress. Water-based ferrofluids present the most complex microstructural behavior and their properties improvement represents an important challenge in this field [1,2].

In the present paper, the structure of a new $CoFe_2O_4$/lauric acid/DDS-Na/H_2O ferrofluid with the particle concentration and temperature variation is investigated by means of small angle neutron scattering (SANS).

Small angle neutron scattering (SANS) measurements of $CoFe_2O_4$/LA/DDS-Na/H_2O ferrofluid samples were carried out using the YUMO instrument installed at IBR-2 high pulsed reactor (JINR, Dubna, Russian Federation), equipped with a two- detector system [3]. The coverage interval of scattering vector Q was $0.006\ A^{-1} < Q < 0.3\ A^{-1}$. The measured neutron scattering spectra were corrected for the transmission and thickness of the sample, background scattering on the film substrate and on the vanadium reference sample using SAS software, yielding a neutron scattering intensity in absolute units of cm^{-1}.

Earlier preliminary results on the transmission electron microscopy (TEM), selected area electron diffraction (SAED) and SANS characterization of the sample were reported [4] (see Figs. 1 and 2).

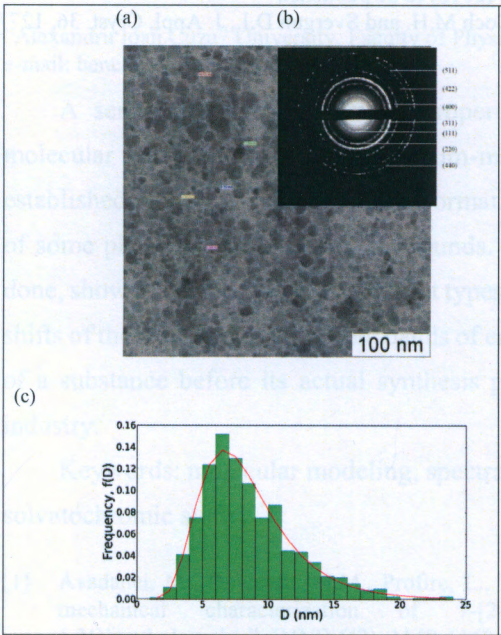

Fig.1 (a) TEM image of: (a) 3% particle vol. concentration $CoFe_2O_4$/lauric acid/DDS-Na/H_2O ferrofluid;(b) selected aria electron diffraction (SAED) pattern of the sample; (c) the size distribution histogram of $CoFe_2O_4$ particles from TEM image [4].

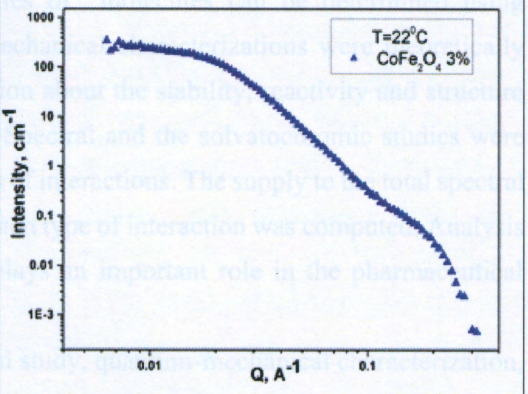

Fig.2 SANS experimental curve of 3% $CoFe_2O_4$/lauric acid/DDS-Na/H_2O particle vol. concentration ferrofluid sample [4].

Results on the structure of diluted samples investigated by SANS at 3 temperature values (22 ^{0}C; 43 ^{0}C; again 22 ^{0}C) are reported in the present work. For obtaining the particle form and structure factors the reduction to zero method (PRIMUS program) is applied [5]. The determined parameters are analyzed and discussed.

Acknowledgements The authors acknowledge the financial support through the grants of the Romanian Governmental Representative at JINR and scientific projects No.95/17.02.2014 items 34, 40, No.96/17.02.2014 items 36, 47 and No.33/23.01.2015 item 59.

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Spectral and quantum-mechanical characterizations of some compounds with biological activity

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A series of physico-chemical properties of molecules can be determined using molecular modeling programs. Quantum-mechanical characterizations were theoretically established and can provide useful information about the stability, reactivity and structure of some pharmaco-therapeutic compounds. Spectral and the solvatochromic studies were done, showing the presence of different types of interactions. The supply to the total spectral shifts of the electronic absorption bands of each type of interaction was computed. Analysis of a substance before its actual synthesis plays an important role in the pharmaceutical industry.

Keywords: molecular modeling, spectral study, quantum-mechanical characterization, solvatochromic study.

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Deterministic mass fractals: a new generating algorithm and structural properties from small-angle scattering

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We suggest a new algorithm for constructing a random mass fractal from a deterministic one. The positions of 'units' inside the fractal are taken at random, while their number is kept constant at each iteration. The small-angle scattering intensity I(q), where q is the scattering vector magnitude, is calculated for a system of randomly oriented fractals with spatially uncorrelated positions. We investigate how the introduced randomness smears the log-periodic function $I(q)q^D$ (D is the fractal dimension) [1] and thus how the scaling factor of fractal can be extracted from the scattering intensity.

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Ferro-magnetic nanoparticles suspensions in twisted nematic cells

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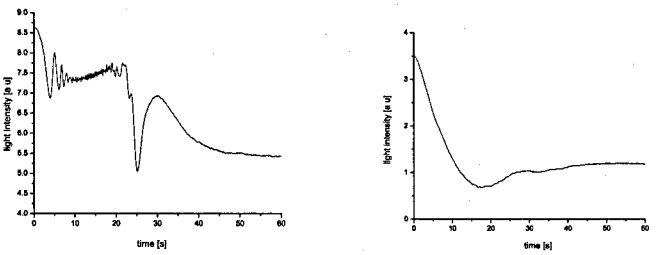
Nanoparticles insertion in nematic liquid crystal cells are used to improve the magnetic [1], electric [2] or electro-optic [3] properties of the mixture. Widely used in electronic devices (LCD-s), where a short reaction time to the external field is required, liquid crystals (LC) also proved to be an important element in unconventional optical component design. In this case, a *stable* structure is preferred to a *rapid* one and, of course, a good optical transparency is also required.

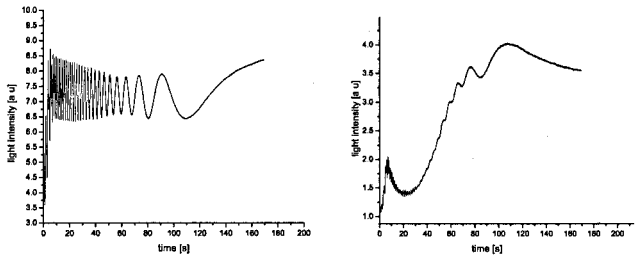
Twisted nematic (TN) effect made LCD-s practical in portable devices taking the advantage of the low power consumption. The main problem of any LCD is the response time of the nematic to the addressing field. When an external magnetic field, higher than the limit for the Freedericksz transition is applied on a nematic liquid crystal cell, it takes about 1min to even 2 or 3 minutes to completely reorient itself to the field depending on its rotational viscosity and elastic constants. During this period, the system is very unstable and the light crossing through it presents a series of maxima and minima before the final state is reached [1].

Our experimental studies revealed that certain magnetic nanoparticles [4] insertion in a TN-cell not only reduces the relaxation time but also changes the mixture into a very stable one, without intermediate oscillations when a magnetic field is suddenly switched on (fig.1) or off (fig.2).



a) *b)*

Fig. 1: Light intensity distribution when a 1050 gauss magnetic field is switched on. a) 5CB TN-cell b)5CB+1%$CoFe_3O_2$ TN-cell



a) *b)*

Fig. 1: Light intensity distribution when a 1050 gauss magnetic field is switched off. a) 5CB TN-cell b)5CB+1%$CoFe_3O_2$ TN-cell

For the TN-cells, glass plates previously prepared for a planar alignment were mounted with the rubbing directions perpendicular to each other and 180 μm Mylar was used to set the thickness. The cells were filled with 5CB nematic from Sigma-Aldrich, for the witness sample, and with a mixture of 5CB and 1% $CoFe_3O_4$ nanoparticles for the studied one. Different magnetic fields (higher than the magnetic Freedericksz transition) were applied on each sample and the laser intensity variation through the cell was recorded.

The results revealed a decrease of the relaxation time, suitable for LCD-s and also an increased stability of the mixture making it properly for LC-based optical compounds.

Acknowledgment:

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The influence of capping agents on the optical and photocatalytical properties of zinc sulfide nanopowders

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Keywords: zinc sulfide, capping agents, optical properties, photocatalyst.

Zinc sulfide is an important II-VI semiconductor, with many aplications in various domains, such as photocatalysis [1], solar cells [2], electronic devices [3] etc. In last years, nanoparticles of ZnS were obtained by various techiques like chemical precipitation [4], hydrothermal method [5], ultrasonic radiation method [6] etc. The synthesis of metal sulfides colloidal nanoparticles typically consists in a reaction of a metal compound with a sulfide ion precursor in the presence of capping agents, which stabilize the high energy surface of the nanoparticles and protect them from aggregation. The role of capping agents in colloidal synthesis of nanoparticles is versatile and must be well understand for catalytic applications of semiconductors. Thus, while the capping agents usually act as a physical barrier to restrict the free access of reactants to catalytic nanoparticles, they can also be utilized to promote catalytic performance of nanocrystals [7]. As well, the capping agents used in the synthesis of semiconductors influence the performances of solar cells based on synthesised semiconductor [8].

We studied the influence of capping agents on the properties of ZnS nanopowders. Therefore, we synthesized ZnS nanopowders using two different capping agents and two experimental techniques. The morphology of nanopowders was studied by transmission electron microscopy and the optical properties were estimated using UV-Visible diffused reflectance spectroscopy; the band gap energy was calculated by Tauc equation from the reflectance spectra. The catalytic activity was determined in the photodegradation of Congo red azo dye. The results were compared with those obtained for bare ZnS nanopowders. The photocatalytic activity of ZnS nanopowder capped with Triton X-100 was remarkably good and superior to ZnS nanopowder capped with polyethylene glycol 200 (PEG 200).

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Risk factors in thermal neutron irradiation on biological systems

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As it is known, any human activity presents some risks. Identify and evaluate risks should be based on professional experience in area of interest. A comprehensive risk information is necessary for any successful risk treatment. So long as the risk are known, deal with it and come up with solutions, under a previously elaborated plan, leads to recover the normal working conditions.

The effect of different radiations on the human subjects is much studied. The paper highlights the action of thermal neutron upon some biological membrane simple models, before and after thermal neutrons irradiation.

The importance of lipids in cell membrane formation and functions is fully recognized [1]. Consequently, we oriented our studies [2] on the behavior of some fatty acids under different external stimuli. Microscopic aspects at the polarizing microscope emphasized liquid crystal smectic C textures for thin film samples up to 25 μm of these systems, between some temperature values. They displayed a thermotropic enantiotropic mesomorphism. In order to avoid parasite effects, the temperature was kept constant by using a digital thermostat designed and realized by us. In electric field of $4x10^4$ V/m the samples behaved as nonlinear dielectrics with a weak conduction.

The action of the thermal neutron irradiation on these substances was studied by using the Ar^+ laser. Under a focused c.w. laser beam, before irradiation, they generally presented a nonlinear optical behavior. An optical hysteresis of the output versus input laser power occurred. After exposed to a flow of thermal neutrons, performed at Bucharest-Magurele, Romania, with a flow of 10-100 meV and 4.15 $x10^{12}$ neutron/cm^2, texture and behavioral changes were noticed. Nonlinear optical effects were evidenced in both saturated and unsaturated samples, but looking different before and after irradiation. We remarked a long time influence of the thermal neutron irradiation upon the long-chain fatty acids. By summarizing the experimental results, we can observe:

For the unsaturated fatty acids, after irradiation textures are unchanged; they present a small hysteretic area for both irradiated and no irradiated samples. Samples with smaller

carbon atom number were more influenced by irradiation. Transmittance was increasing with carbon atom number, on the opposite with the saturated acids; transmittance increased for the irradiated samples.

For the saturated fatty acids: Some irradiated acids present colored regions between perpendicular nicols, which disappeared at parallel nicols. Transmittance was higher for the irradiated samples and increased with the carbon atom number decrease. Hysteresis area decreased with the carbon atom number increasing; the sense of the hysteretic curve is in general the same for all samples, except the situations when, at very low incident laser powers some oscillations appeared.

After a month, saturated acid samples seemed to come back to the initial state and behavior. A second irradiation, applied after 3 month, had a similar effect like the first one. After one year, these samples were again investigated with the same experimental installation and some results are illustrated in the paper. We believe that irradiation induced a shift of the molecules from the smectic plane and changed the electric state of the samples. Also the length of the molecule is important in saturated acids and the distance between the double bound and the carboxyl group in unsaturated ones.

These changes could be evidenced by the nonlinear optical answer of the samples under low power, undestructive, laser light. These observations evidenced that thermal neutrons irradiation influences the fatty acids, components or forerunner of the biological membrane, and this could be studied by using low power laser technologies.

Taking into account this risk, a predictive and quantitative picture of management of the risks must be elaborated and a strategy against must be prepared [3]. This process is computer modeled in the paper by a nonlinear equation, for obtaining a stable output after risks treatment.

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Neutron depolarization investigations of spring exchange interaction nanocomposites

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Neutron depolarization of magnetic state of spring exchange interaction nanocomposites based on NdFeB is carried out. It is detected a different behavior for magnetically soft and rigid nanocomposite. Magnetically hard nanocomposite exhibits coercive force equal to field of maximal neutron depolarization and for soft one a maximal depolarization field has value smaller than coercive field. Conclusion is made that it is connected with different magnetization regime and it is important for realization of spring regime. It was carried out also magnetic measurements using vibrating sample magnetometer and X-ray diffraction in order to evaluate the crystallographic phases involved in relationship with the magnetic behavior.

A case study of the transport processes of tropospheric aerosols over the Ciric-Iasi leisure area

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This paper presents a case study based on monitoring of tropospheric aerosols in correlation with meteorological regional data in the period January – May 2015. Moreover, some water and soil tests were also performed to obtain a thorough characterization of the Ciric Area.

This area of water accumulation prints its mark on the elements and weather phenomena, consisting of lower temperatures, higher humidity, air masses descent, the increased effect of the wind due to the flat surface, radiation and evaporation fog, more pronounced cloudiness, local rainfall, changes in desiccation.

The diurnal effect is noticeable through overnight heating and cooling during the day. The long-term monitoring will contribute to highlighting the variations of meteorological parameters due to the cold to hot season transition. In the short term, we are also expecting to see variations for tropospheric pollutants and those from the soil and water.

The data from particulate matter (PM) monitoring show frequent breaches of limit values, while those of tropospheric ozone concentrations have been not exceeded. As an immediate impact we are expecting that, due to the increase in the anthropogenic influences over this area, all monitored parameters will change.

Meteorological and AERONET data were also taked into account, for complementary studies regarding aerosol classification and its regional influences. Some optical parameters, like Angstrom coefficients and Single Scattering Albedo show a load of urban/industrial aerosol with slight influence of biomass burning from January to May 2015.

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Environmental fingerprint of human activities revealed by analysis of solid sludges from waste water treatment plants

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The analysis of sludges samples collected from different waste water treatment stations is important not only for monitoring the correct operation of the plant but also it enables to monitor the environmental impact in the area of that station. Elemental analysis techniques EDXRF, AAS, INAA were used to characterize the chemical composition of the analyzed materials. Thermal analysis (DSC) was applied to characterize the thermal behavior and the organic content while ATR-FTIR was used to provide data about both the molecular nature of organic component and the structure of inorganic phase. The experimental results revealed significant differences concerning both the content of heavy metals and organic compounds. A tentative to correlate the chemical features of sludges to dominant activities in the monitored area of each treatment plant is presented. Hence it becomes possible to depict an image of the environmental impact of human activities in a certain area as exemplified here for Targoviste and surroundings.

2D fractional brownian motion simulation of COFE2O4/DBS-DBS/H2O ferrofluid anizotropy

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We present SANS measurements on CoFe2O4/DBS-DBS/H2O ferrofluid samples subjected to temperatures in the range of 10 – 60^0 C and preliminary studies of surface anisotropy based on 2D fractional Brownian motion (2DfBm) simulation.

For increasing and decreasing temperatures, SANS curves show almost similar shapes except small deviations in the limits below 0.01 A^{-1} and above 0.1 A^{-1} (Fig.1).

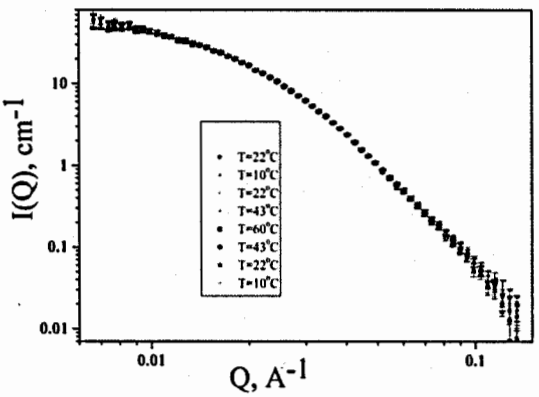

Fig. 1 SANS experimental curves of CoFe2O4/DBS-DBS/H2O sample at different temperatures.

This demonstrate a good stability of the investigated probe. The magnetic fluid under study was supplied by the Laboratory of Magnetic Fluids at the Center of Fundamental and Applied Research of the Romanian Academy of Sciences Timisoara, Romania.

Previous study on a similar fluid established that SANS curves could be effectively used to study clusters kinetic changes in aqueous magnetic fluids under different conditions [1]. The scattering intensity profile shows, in certain intervals of the scattering vector Q, a power law dependence: $I(Q) = I_0 Q^{-\alpha}$, indicating fractal nature of structures. For $2<\alpha\leq 3$, a mass fractal is defined with the fractal dimension $D_m = \alpha$ whereas for $\alpha > 3$, a surface fractal with dimension $D_s = 6 - \alpha$ is used [2-5]. These values can be correlated with corresponding Hurst exponent $H = d + 1 - D$, where d is the dimension of the supporting space. If the Hurst exponent is different from 0.5, the surface is known as Brownian and it can be modeled as a 2D Brownian surface. $H < 0.5$ corresponds to a fragmented surface with many small irregularities while $H > 0.5$ describe a smoother

surface. Using the 2D fractional Brownian surface simulations for particular values of H and the tensor of gyration, we measure the anisotropy of the spatial arrangement of the ferrofluid particles and clusters.

Acknowledgements: This study is supported by JINR-UPB Project No 33/23.01.2015 item 46 and Project No.34/23.01.2015 item 45.

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Double layers of anisotropic materials cut parallel to optical axis, between crossed polarizers

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Two anisotropic uniax layers cut parallel to their optical axis and having known thicknesses are used between crossed polarizers in order to determine the linear birefringence, its dispersion and the order of channels from channeled spectra. The method is very useful for the determination of the birefringence of the thin anisotropic films, for which channeled spectra can not be obtained. Two channeled spectra were recorded for the two anisotropic layers having the optical axes parallel and perpendicular.

Keywords: anisotropic uniax layers, channeled spectrum, linear birefringence, dispersion of linear birefringence, order of channels.

Small-angle neutron scattering (SANS) investigation on titanium based composites deposited by thermionic vacuum arc (TVA) method

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Thin film deposition process by thermionic vacuum arc (TVA), an original discharge type in pure vapor plasma, might become one of the most suitable technologies to significantly improve the tribological properties of the surfaces covered with different materials. Due to the deposition in high vacuum conditions and without buffer gas the films have a high purity, increased adhesion, low friction, low roughness, and a compact nanostructure. In this study, we report for the first time a small-angle neutron scattering (SANS) investigation of the titanium based materials deposited on different substrates and conditions by the TVA method. Titanium based thin films are envisaged for surface coatings applications requiring low roughness, good smoothness and low friction coefficient.

Small-angle neutron scattering (SANS) is a valuable technique for studying nanostructures, which characteristic structural features lies mostly in the interval of 1-100 nm. For instance, Fig.1 gives the scattering curve from Ti-Ag deposited on a special substrate required by specific industrial applications (OLC 45-stainless steel with 45 percent of carbon inside).

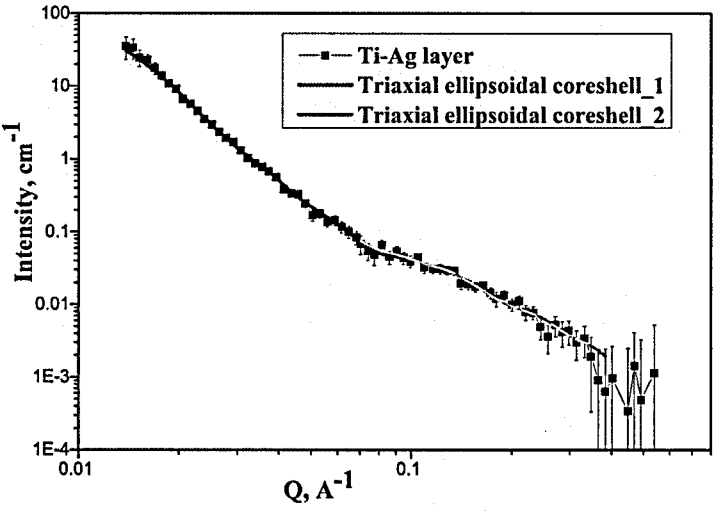

Fig.1 SANS from Ti-Ag layer and the model curve fittings with FITTER program: (i) experimental data in the range of 0.01 $Å^{-1} \leq Q \leq 0.3$ $Å^{-1}$ (black squares); (ii) triaxial ellipsoidal coreshell fit (red line): another triaxial ellipsoidal coreshell fit (green line)

The preliminary investigations have shown that the characteristic SANS contribution from the Ti-Ag layer in the range of 0.01 $Å^{-1} \leq Q \leq 0.3$ $Å^{-1}$ reveals different sized nanostructures (see Fig.1). This result indicates promising perspectives for future investigations.

For another titanium based composite series such as Ti-C, there were not detected differences between the curves from deposited TiC/OLC 45 layers. The curves present just the scattering characterizing the substrate. The influence of the thickness as well as the interface between the deposited film and the substrate are of great importance for this study.

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