

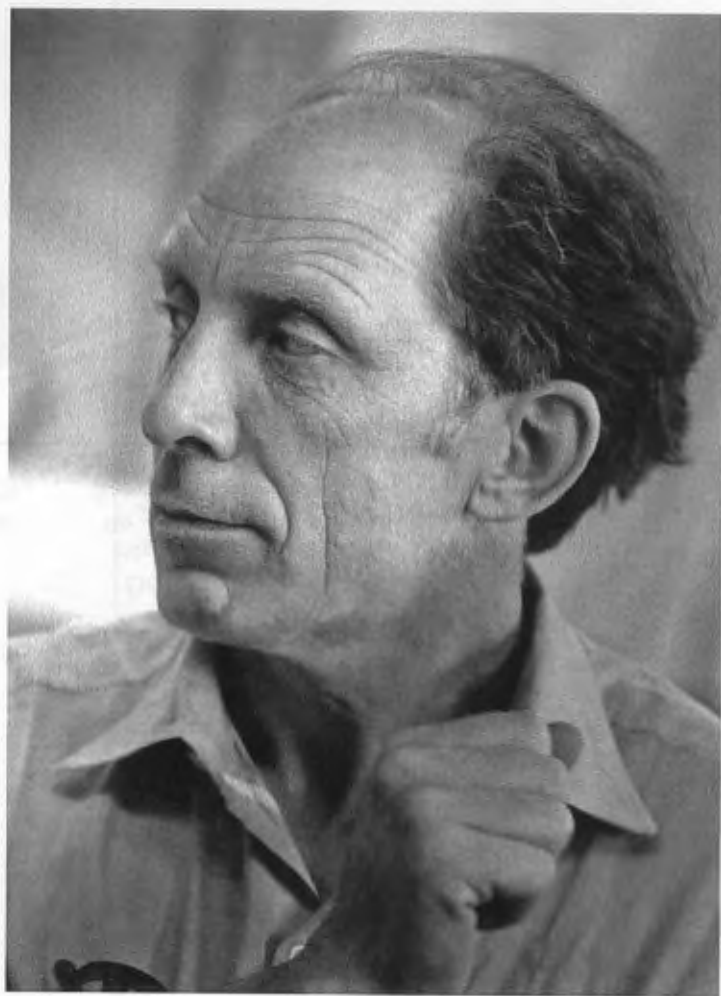
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**III INTERNATIONAL CONFERENCE
ON SMALL ANGLE NEUTRON SCATTERING
DEDICATED TO THE 80TH ANNIVERSARY
OF YU. M. OSTANEVICH**

Book of Abstracts





ЭКЗ. ЧИТ. ЗДР

Joint Institute for Nuclear Research
Frank Laboratory of Neutron Physics

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Dubna, June 6–9, 2016

Book of Abstracts

Dubna•2016

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БИБЛИОТЕКА
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Alexander I. Kuklin, Norbert Kučerka, Maria Balasoiu, Oleksandr I. Ivankov

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Contents

Contents	4
Preface	13
Keynote Speakers	15
E. Burzo	
<i>Exchange interactions in heavy rare earths RCo₂ compounds</i>	16
J. Katsaras	
<i>Biomembranes Research at ORNL: in search of nanoscopic lipid domains in model and bacterial membranes</i>	18
A. Michels	
<i>Magnetic SANS on bulk ferromagnets</i>	19
A.N. Ozerin, T.S. Kurkin, O.V. Lebedev, E.K. Golubev	
<i>Polymer-Nanoparticles Composites. Quo Vadis?</i>	21
O. Zimmer, H.M. Jouve, H.B. Stuhmann	
<i>Polarised proton spin density images tyrosyl radical locations in bovine liver catalase</i>	22
J. Teixeira	
<i>The contribution of small angle scattering to the physics of liquid water</i>	24
N.R. Zaccai	
<i>Skipping between Portals: Neutron analysis of membrane protein biogenesis</i>	25
Invited Speakers	
G.M. Arzumanyan	
<i>Raman, CARS and SERS spectroscopy and microscopy: modern challenges and some applications</i>	28
M.V. Avdeev	
<i>Small-angle neutron scattering in structural research of detonation nanodiamonds</i>	29
L. Cser	
<i>Neutron holography</i>	31
W. Gille	
<i>Small-Angle Scattering of spheres: results for small volume fractions and special pair correlations</i>	32

F. Iacomi

- Studies on some iron oxide nanoparticles, nanocomposites
and thin films for advanced applications* 34

G.N. Rychkov, A.V. Ilatovskiy, I. Nazarov, A. Shvetsov, D. Lebedev,
A. Konev, V. Isaev-Ivanov, A.V. Onufriev

- Partially assembled nucleosome structures at atomic detail* 36

J. Jestin, S. Désert, R. Hanslik, S. Jaksch, H. Frielinghaus

- The Small-K Advanced Diffractometer SKADI, a multi-purpose SANS instrument
at ESS for high impact science in soft matter and biological systems* 37

P. Kopcansky, L. Balejckikova, M. Molcan, M. Timko, K. Siposova, O. Strbak,
M.V. Avdeev, V.I. Petrenko, V.M. Garamus, L. Almasy, K. Pospiskova, I. Safarik

- The structural study of magnetoferritin and its complex systems
by means of SAXS and SANS* 38

N. Kučerka

- Condensed Matter Research at Frank Laboratory of Neutron Physics* 40

V.T. Lebedev

- Small angle neutron and X-ray studies of carbon structures with metal atoms* 41

Runov V.V.

- Nuclear-magnetic interference effects in small-angle scattering
of polarized neutrons* 43

D. Uhríková, J. Teixeira, L. Hubčík, A. Búcsi, T. Kondela, T.N. Murugova,

O.I. Ivankov

- Lipid based drug delivery systems: Kinetics by SANS* 44

R. Vladioiu, A. Mandes, V. Dinca-Balan, G. Prodan

- Nanostructured titanium based materials synthesized
by Thermionic Vacuum Arc (TVA) method for industrial applications* 45

V.V. Volkov

- Size and Structure Characterisation of Nanoparticles
by Small-Angle Scattering: Uniqueness, Reliability, Methods* 47

Contributed Talks

E. Puscasu, L. Sacarescu, N. Lupu, M. Grigoras, M. Balasoioiu, D. Creanga

- Iron oxide nanostructures – investigation of microstructural
and magnetic properties* 50

Contents

O.I. Ivankov, D.V. Soloviov, A.V. Rogachev, Yu.S. Kovalev, A.P. Sirotn, A.S. Kirilov, T.B. Petukhova, A.G. Soloviev, T.M. Solovjeva, A.I. Kuklin	
<i>Small angle scattering instrument YuMO</i>	51
Yu.V. Kulvelis, S.S. Ivanchev, O.N. Primachenko, V.T. Lebedev, A.I. Kuklin	
<i>Fine structure and performance of perfluorinated proton conducting membrane systems</i>	52
Yu.V. Larichev	
<i>Application masking liquid technique for SAXS study of nanocomposites</i>	54
D.V. Lebedev, R.A. Pantina, M.V. Filatov, V.V. Isaev-Ivanov	
<i>Effect of molecular crowding modulating agents on chromatin structure revealed by SANS</i>	55
V.S. Molchanov, A.L. Kvyatkovsky, O.E. Philippova	
<i>Cylindrical flexible micelles of ionic surfactant produced by nonorganic salts</i>	56
K.A. Motovilov, A.A. Pronin, E.S. Zhukova, Z.V. Gagkaeva, V.I. Torgashev, M. Savinov, V. Grinenko, M.A. Belyanchikov, A.K. Grebenko, M.A. Letarova, K.V. Sidoruk, T.N. Murugova, O.I. Ivankov, M. Dressel, B.P. Gorshunov	
<i>Dielectric Universalities and Charge Transport in Bacterial Filaments: Structural Data from SANS</i>	58
M.A. Ostrovsky, T.B. Feldman, O.I. Ivankov, T.N. Murugova, A.I. Kuklin, M.A. Yakovleva, V.I. Gordeliy, A.V. Belushkin	
<i>Study of visual pigment rhodopsin supramolecular organization in photoreceptor membrane by SAXS and SANS</i>	60
V.N. Pribora	
<i>Bruker SAXS Solutions</i>	61
A.V. Shibaev, A.V. Rogachev, A.I. Kuklin, O.E. Philippova, A.R. Khokhlov	
<i>Small-angle neutron scattering study of hydrocarbon-responsive surfactant micellar networks</i>	63
A.A. Shiryayev, V.V. Volkov, P. Pré, A.M. Voloshchuk	
<i>Structure of Nanoporous Carbons as revealed by Small-Angle X-Ray Scattering and TEM</i>	65
A.V. Shvetsov, M.A. Koltsov, D.V. Lebedev, V.V. Isaev-Ivanov	
<i>How to get D₂O/H₂O contrast estimation from all-atom molecular dynamics trajectories for large biomacromolecular complexes</i>	67

O.V. Tomchuk, M.V. Avdeev, L.A. Bulavin	
<i>Fractal aggregates of polydisperse particles with tunable dimension</i>	69
A.N. Zhigunov, P. Matejcek	
<i>Small angle and wide angle x-ray scattering study of boron clusters: interparticle correlations</i>	71
Poster Session	
L. Anghel, R.V. Erhan	
<i>Beta-lactoglobulin self-assembly: a small angle neutron scattering study</i>	74
D. Arangel, C.R. Badita	
<i>Measurements on the collagen by neutron contrast variation</i>	75
V.Y. Bairamukov, V.T. Lebedev, V.I. Tikhonom	
<i>SANS-study of carbon matrices made by pyrolysis of bis-phthalocyanines of metals used for storage and transmutation of radioactive waste</i>	77
M. Balasoiu, S.V. Kozhevnikov, Yu.V. Nikitenko, I. Bica, M. Bunoiu	
<i>Neutron depolarization method applied for magnetorheological elastomers investigations</i>	79
S.E. Kichanov, M. Balasoiu	
<i>Synchrotron powder diffraction investigations of biogenic ferrihydrite particles transformations induced by variation of the growth conditions for the microorganisms</i>	81
M. Balasoiu, V.T. Lebedev, I. Bica, M. Bunoiu, A.V. Rogachev	
<i>SANS investigation of magnetic polydimethylsiloxane elastomers polymerized in different oriented magnetic fields</i>	83
R. Vladoiu, M. Balasoiu, D. Soloviov, A. Mandes, V. Dinca	
<i>SANS investigations of Ti-Ag thermionic vacuum arc deposition</i>	85
M. Balasoiu, D.V. Soloviov, A.-M. Balasoiu-Gaina, O.I. Ivankov, N. Lupu	
<i>Concentration effects in cobalt ferrite/lauric acid-sodium dodecyl sulphate/water ferrofluid studied by means of SANS</i>	87
V. Bodnarchuk, O. Pana, M. Rada, R.V. Erhan, R.-C. Suci, N. Aldea,	
C. Leoştean, S. Rada, A. Kuklin	
<i>Structural studies using small-angle neutron scattering of germane-lead glasses doped with silver oxide</i>	90

Contents

N.V. Bulat, L.A. Avakyan, V.V. Pryadchenko, V.V. Sraibonyan, S.V. Belenov., L.A. Bugaev	
<i>Study of carbon-supported bimetallic PtCu nanoparticles by ASAXS</i>	91
I.M. Byvshev, I.M. Vangeli, T.N. Murugova, O.I. Ivankov, A.I. Kuklin, V.I. Popov, V.V. Teplova, L.S. Yaguzhinsky	
<i>Ultrastructure of heart mitochondria studied by SANS and SAXS</i>	92
A.C. Dragolici, M. Balasoiu, F. Dragolici, L. Ionascu, M. Micu, O.I. Ivankov	
<i>SANS investigations of special aluminous cement matrices for conditioning of radioactive waste</i>	94
L. Anghel, R.V. Erhan	
<i>Hetero-association of beta-lactoglobulin and sodium alginate studied by small-angle neutron scattering</i>	96
R.V. Erhan, M. Rada, R.-C. Suci, M. Zagrai, S. Rada, E. Culea, C. Leostean, N. Aldea	
<i>Small-angle neutron scattering structural investigation of porous ceramic glasses</i>	97
A. Gapchenko, A. Vlasov, Yu. Ryzhykau, E. Zynoviev, Yu. Kovalev, V. Borshchevskiy, V. Gordeliy, A. Kuklin	
<i>Analysis of M-state of Bacteriorhodopsin D96N</i>	99
I.V. Gapon, V.I. Petrenko, L.A. Bulavin, A.A. Vorobiev, O. Soltwedel, M. Balasoiu, L. Vekas, V. Zavisova, P. Kopcansky, M.V. Avdeev	
<i>Structure stability of magnetic fluids in bulk and interfaces: combined analysis of small-angle neutron scattering and neutron reflectometry</i>	100
C. Chilom, D. Gazdaru, G. Socol, A. Popescu, M. Balasoiu	
<i>Spectroscopic studies on biogenic ferrihydrite nanoparticles produced by bacteria Klebsiella oxytoca</i>	102
W. Gille, S. Ciccariello	
<i>The intersect distribution of the tetrahedron: Approaches for simplification of cyclometric terms</i>	103
T.L. Hangan, D. Badiu, S. Vladareanu, D. Navolan	
<i>The role of small angle neutron scattering technique in transdermal drug delivery</i>	105
R.F. Hashimov, E.B. Askarov, A.I. Beskrovniy, D.N. Toan, S.H. Jabarov, D. Neov, E.M. Karimova	
<i>Neutron diffraction study of the crystal and magnetic structures of $TiFe_{1-x}Ga_xS_2$ compounds</i>	106

I. Ion, M. Lungu, V. Marinescu, D. Patroi, M. Lucaci, V. Thakiris, E. Mantea, M. Balasoïu, Yu.S. Kovalev, A.I. Kuklin, Yu. Nikitenko	
<i>Multifunctional Composite Materials</i>	108
A.S. Kazantsev, A.V. Vlasov, Yu.L. Ryzhykau, O.I. Ivankov, D.V. Soloviov, E.V. Zinovev, A.V. Rogachev, Yu.S. Kovalev, V.I. Gordeliy, A.I. Kuklin	
<i>Silver behenate and silver stearate for better Q-scale SAS calibration</i>	110
S.E. Kichanov, V.S. Gurin, D.P. Kozlenko, O.I. Ivankov, A.Kh. Islamov, G.E. Rachkovskaya, B.N. Savenko	
<i>Optical active nanoparticles in a silicate glasses: SANS studies.</i>	111
T. Kondela, J. Gallová, T. Hauss, N. Kučerka, O.I. Ivankov, P. Balgavy	
<i>Effect of alkan-1-ols on the structure of DOPC model membrane</i>	113
N.N. Gubanova, G.P. Kopitsa, A.E. Baranchikov, V.K. Ivanov	
<i>Transparent zirconia classes: synthesis, structure and optical properties</i>	114
A.P. Luginina, A.Yu. Gusach, A.V. Mishin, N.A. Vartanyan, R.O. Astashkin, A.O. Bogorodskiy, M.M. Ergasheva, V.I. Borshchevskiy, V. Cherezov	
<i>Human CysLT1 expression, purification, crystallization</i>	115
A. Dumbrava, G. Podan, F. Moscalu	
<i>Synthesis and Characterization of PEGylated Zinc Sulfide Nanopowders</i>	116
A.A. Nabiev, A.M. Maharramov, A.I. Kuklin, E.B. Asgerov	
<i>Small angle neutron scattering study of high-density polyethylene zirconium oxide nano composites</i>	118
L. Oprica, M. Andries, I. Bodale, M. Balasoïu, D. Creanga	
<i>Magnetic nanoparticle properties studied with condensed matter methods and biochemical assays</i>	119
A.-M. Putz, L. Almásy, A. Len, C. Ianăși, J. Pleštil, C. Savii	
<i>Mesoporous silica prepared using a pyridinium ionic liquid and studied by small angle scattering</i>	120
A. Rajewska, A.Kh. Islamov	
<i>SANS method study of surfactant mixture system nonionic+anionic in heavy water solutions</i>	121

Contents

A.D. Rogov, O.I. Ivankov, D.V. Soloviov, Yu.S. Kovalev, A.V. Rogachev, R.V. Erhan, A.I. Kuklin	
<i>The fluxes of cold and thermal moderator at 4-th beam-line:</i>	
<i>Monte-Carlo simulation and experiments</i>	122
K. Rečko, J. Waliszewski, U. Klekotka, D. Satuła, F. Damay, M. Biernacka, M. Balasoiu, K. Szymański	
<i>Properties of the magnetic nanoparticles of gallium ferrites and ferrofluids</i>	123
M.I. Rulev, D.V. Zabelskii, A.V. Vlasov, D.V. Soloviov, O.I. Ivankov, Yu.L. Ryzhykau, E.V. Zinovev, V.I. Gordeliy, A.I. Kuklin	
<i>Lipidic membranes structural conformations in aqueous solutions from SAXS and SANS comparative analysis</i>	125
M.I. Rulev, O.I. Ivankov, D.V. Soloviov, D.V. Zabelskii, A.V. Vlasov, Yu.L. Ryzhykau, E.V. Zinovev, N. Kučerka, V.I. Gordeliy, A.I. Kuklin	
<i>Investigations of the phase transition of DPPC MLVs co-dispersed in water solution with potassium chloride</i>	126
Yu.L. Ryzhykau, M.Yu. Nikolaev, D.V. Soloviov, O.I. Ivankov, Yu.S. Kovalev, T.N. Murugova, E.V. Zinoviev, A.V. Vlasov, A.V. Rogachev, V.I. Borshchevskiy, V.I. Gordeliy, A.I. Kuklin	
<i>About the possibilities of Small Angle Scattering method: applications to nanodiscs structure studies</i>	128
V.V. Sadilov, V.I. Bodnarchuk, S.A. Manoshin, R.V. Erhan, A. Ioffe	
<i>Monte Carlo simulation of SESANS experiment with time-gradient magnetic fields</i>	130
D.V. Seliverstova, O.I. Ivankov, T.N. Murugova, D.V. Soloviov, A.I. Kuklin, V.I. Gordeliy	
<i>The investigation of the structure of bicelles by small-angle scattering method</i>	131
D.B. Shemet, V.V. Pryadchenko, V.V. Srabionyan, S.B. Belenov, L.A. Avakyan, V.E. Guterman, L.A. Bugaev	
<i>The effect of thermal treatment on the atomic structure of PtCu core-shell nanoparticles in PtCu/C electrocatalysts</i>	133
A.P. Sirotnin, A.S. Kirilov, T.B. Petukhova, D.V. Soloviov, O.I. Ivankov, A.I. Kuklin	
<i>Modernization of the control motors and sample environment system of YuMO spectrometer at IBR-2M</i>	135

A.Y. Sluchevsky, D.V. Soloviov, M.I. Rulev, A.I. Kuklin <i>Small-angle neutron scattering study of phase transitions of mixed lipid membranes in water solution</i>	136
R. Smyslov, G. Kopitsa, Yu. Gorshkova, O. Ivankov, K. Ezdakova, Yu. Chetverikov, A. Bugrov, A. Zavialova, A. Khripunov, A. Tkachenko, V. Haramus, B. Angelov, V. Pipich, N. Szekely <i>Structural morphology of Gluconacetobacter xylinus cellulose, and of organo-inorganic composite materials on its base</i>	138
A.G. Soloviev, O.I. Ivankov, D.V. Soloviov, A.V. Rogachev, Yu.S. Kovalev, T.M. Solovjeva, A.I. Kuklin <i>SAS program: current status and future</i>	139
A.V. Rogachev, A.G. Soloviev, O.I. Ivankov, D.V. Soloviov, T.M. Solovjeva, A.I. Kuklin <i>Corporate information system for development of SANS software</i>	140
M. Balasoiu, O.I. Ivankov, C. Stan, D. Buzatu, C.P. Cristescu <i>Fractal analysis of CoFe₂O₄/lauric acid/DDS-Na/H₂O ferrofluid from TEM and SANS measurements</i>	142
M.V. Suyasova, Yu.V. Kulvelis, V.T. Lebedev, A.A. Szhogina, V.P. Sedov, A.I. Kuklin <i>Self-assembly of endofullerenol-water systems</i>	144
A.V. Vlasov, Yu.L. Ryzhykau, E.V. Zinoviev, D.V. Soloviov, O.I. Ivankov, P.K. Utrobin, A.V. Mishin, V.I. Gordeliy, V.I. Borshevskiy, A.I. Kuklin <i>Small-angle scattering sheds light on dimerization mechanism of iron-regulating protein apoferritin</i>	146

Authors list

Keynote Speakers	147
Invited Speakers	147
Contributed Talks	147
Poster Session	148
Authors List	149

Contents

Last minute abstracts

Yu.S. Kovalev, D.V. Soloviov, O.I. Ivankov, A.V. Rogachev, A.V. Vlasov, Yu.L. Rzyzhkau, E.V. Zinovev, P.K. Utrobin, V.I. Borshevskiy, V.I. Gordeliy, A.I. Kuklin	
<i>Small-angle X-ray pinhole camera system Rigaku: parameters and first results</i>	153
A.Yu. Cherny	
<i>The structure of deterministic mass, surface and multi-phase fractals from small-angle scattering data</i>	154
V.V. Yegorov, D.V. Lebedev, Y.A. Yagudina, A.I. Kuklin	
<i>Oligomerization of the ionic self-complementary peptide study</i>	155
J. Waliszewski	
<i>Magnetization distribution in non-collinear systems. The method</i>	156
D.M. Chudoba, Yu.E. Gorshkova, I. Zinikovskaia	
<i>FLNP JINR User Program</i>	158

Preface

III International Conference on Small Angle Neutron Scattering is taking place at the Frank Laboratory of Neutron Physics of the Joint Institute for Nuclear Research in Dubna on June 6-9, 2016.

The conference is the 3rd continuation of a successful series of scientific meetings dedicated to Yuriy Mechislavovich Ostanevich (1936–1992), who was the founder of small-angle neutron scattering (field, group, and instrument) at the FLNP. He contributed in particular, to the development of time-of-flight SANS technique, and the selection of advanced scientific areas for its application. The modern SANS instrument at the FLNP is named YuMO in his honour, while a number of awards including the State Prize of the Russian Federation in 2000 recognize his leadership and outstanding scientific achievements in SANS studies of polyelectrolytes, small molecules, fractals, metallic glasses, macromolecules, polymers, etc. This year we celebrate the 80-th anniversary of this outstanding neutron physicist.

More than 40 years ago, the first SANS instrument on a steady-state reactor was constructed at the Institute Laue Langevin, Grenoble, while the first SANS instrument on a 'white' neutron pulsed beam was assembled at the Joint Institute for Nuclear Research at the reactor IBR-30. The SANS technique has ever since been applied to a wide range of scientific problems in condensed matter, soft matter, biology, and nanotechnology. Despite the fact that there are currently over 30 SANS instruments in operation worldwide, at both reactor and spallation sources, the demand for beam-time is considerably higher than the time available.

The first SANS-YuMO meeting was held in October 2006. Research groups from different neutron centers, universities and research institutes across Europe presented more than 35 oral and poster contributions describing various scientific and methodological results. The most of them were obtained using the SANS-YuMO instrument installed at the high-flux pulsed reactor IBR-2.

The second event was organized in June 2011, conveniently at the start-up of the scientific experiments after the IBR-2 refurbishment and accomplishment of comprehensive modernization (2006-2011). It had brought together many leading scientists of small-angle neutron scattering and soft condensed matter research coming from 12 countries comprising Czech Republic, Egypt, France, Germany, Hungary, Moldova, Mongolia, Poland, Romania, Russian Federation, Slovak Republic, and Ukraine. The participants had a chance to listen to 27 oral talks and to view 32 posters.

Preface

The increasing amount of interest to participate to these events and to present own scientific results in the field of SAS and its complimentary methods, biology, magnetic, polymers, colloids and other systems of condensed matter prompted us to continue and extend the tradition. We are very pleased to welcome you to the III International Conference on Small Angle Neutron Scattering at the Frank Laboratory of Neutron Physics of Joint Institute for Nuclear Research in Dubna!

Alexander Kuklin, Maria Balasoiu, Norbert Kučerka

KEYNOTE

SPEAKERS

Exchange interactions in heavy rare earths RCO_2 compounds

E. Burzo

Faculty of Physics, Babes-Bolyai University 40084 Cluj-Napoca, Romania

A model is developed in order to describe the magnetic behaviour of ferrimagnetic RCO_2 compounds, at $T > T_c$, in correlation with the exchange interactions. The exchange interactions between R and Co are of 4f-5d-3d type, while those of Co3d-Co3d or R5d-R5d are of short range. A minor contribution of RKKY-type can be also present. The R5d band polarization is a key point in analysing the magnetic behaviour of RCO_2 compounds. This is determined by both local 4f-5d exchange, $M_{5d}(f)$, as well as by R5d-Co3d short range exchange interactions, $M_{5d}(d)$ [1]. At the level of the unit cell, these interactions are interdependent, at equilibrium determining both the cobalt moment as well as the R5d band polarization.

The polarized neutron diffraction measurements, at $T > T_c$, in the presence of an external field, evidenced an antiparallel coupling of M_R and M_{Co} moments [2]. The analysis of the above data shows a linear dependence of cobalt moments as function of the rare-earth ones, the slopes

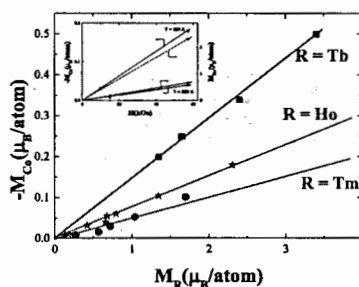


Fig.1

being dependent on the R atom magnetization— Fig.1. Short range correlations at $T_c < T \leq T_J$ were evidenced by a SAS experiment on ErCo_2 , the correlation length being of 7-8 Å [3], close to the lattice parameters of RCO_2 compounds $a \approx 7.2$ Å. The above correlations were attributed to a remanent magnetic ordered phase (Griffith phase), at $T > T_c$. This phase was considered to be at

the origin of the antiparallel coupling of R and Co moments above T_c , behaviour, called parrimagnetism [2].

Both polarized neutron studies as well as magnetic measurements suggest that at $T > T_c$ the system behaves as a paramagnet. As example, M_{Co} is linearly dependent on external field – Fig.1 as well as the magnetic susceptibilities χ . In addition the χ values show a nonlinear temperature dependence typical for a ferrimagnetic system. The slopes a of M_{Co} vs. M_R plots follow the same

trend as R5d band polarization, - Fig.2 - evidencing that the 4f-5d-3d (3d-3d, 5d-3d) still exist above T_c , but the exchange interactions intensities are rather low.

The sublattice coupling can be shown only in the presence of external field. Even in the LuCo_2 exchange enhanced paramagnet, in a field of 5.7 T at 100 K, an induced cobalt moment, antiparallel oriented to Lu5d band polarization has been observed. The electronic contribution to the specific heat can be described, at $T_c < T < 300$ K by a relation $C(T)/T = a + b\sqrt{T}$ compatible with 3d-SDW QCP model.

The present model associates the cluster dimensions, evidenced by SAS data, with that of the RCO_2 unit cell, where all the magnetic atoms are magnetically coupled in the paramagnetic phase, the exchange interactions being not enough to induce a magnetic order. A parallel alignment of M_{Co} and M_{R} , in the presence of the external field can be seen at temperatures $T > T_c$, where the thermal energy is higher than that involved in magnetic couplings. The thermal evolution of cobalt moment, which increases with temperature, as predicted by spin fluctuation model, contributes to a more complex magnetic behaviour at $T > T_c$.

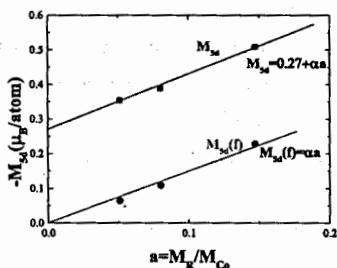


Fig.2

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Biomembranes Research at ORNL: in search of nanoscopic lipid domains in model and bacterial membranes

J. Katsaras

Oak Ridge National Laboratory, 37831 Oak Ridge, USA

katsarasj@ornl.gov

Biomembranes are the active boundary between cells and their surroundings. They are sophisticated and dynamic machines that perform a diverse array of functions, including selective transport, localization, communication and recognition, to name a few. It is also widely accepted that the plasma membrane is laterally heterogeneous, containing nanoscopic regions enriched in lipids which have different physical properties from their surrounding lipids. These functional lipid domains are commonly referred to as "rafts". Rafts have been implicated in a wide range of cellular functions, including signal transduction, drug uptake, and interactions with pathogens. In recent years, we have used small angle neutron scattering (SANS) to study nanoscopic lipid domains in model membrane systems [1-3], and more recently in the Gram-positive bacterium *Bacillus subtilis*. Data from these studies will be presented, including SANS data from bacterium's membrane under *in vivo* conditions.

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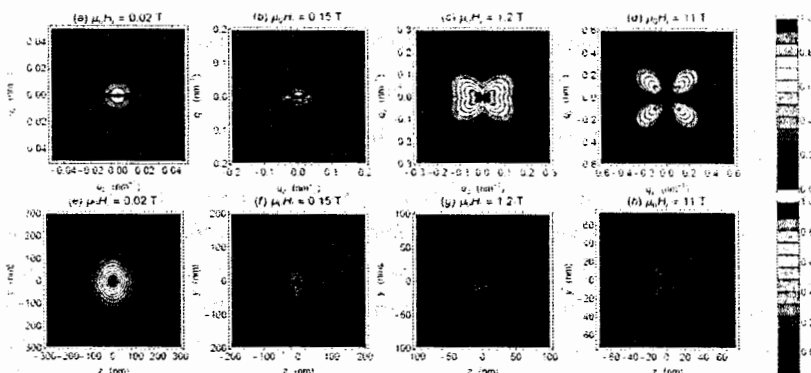
Magnetic SANS on bulk ferromagnets

A. Michels

Physics and Materials Science Research Unit, University of Luxembourg
andreas.michels@uni.lu

Small-angle neutron scattering (SANS) is a very powerful technique for the investigation of magnetic materials, since it provides information from within the *bulk* of magnetic media and on a length scale between a few nanometers and a few hundred of nanometers ($\sim 1\text{-}300\text{ nm}$). In this talk, we summarize recent theoretical and experimental work in the field of magnetic SANS of bulk ferromagnets [1]. The response of the magnetization to spatially inhomogeneous magnetic anisotropy and magnetostatic stray fields is computed using micromagnetic theory, and the ensuing spin-misalignment SANS is deduced. This approach – originally pioneered by Kronmüller, Seeger, and Wilkens [2] – goes beyond the traditional description of SANS in terms of particle form and structure factors. Analysis of experimental magnetic-field-dependent SANS data corroborates the usefulness of the approach, which provides important quantitative information on the magnetic-interaction parameters such as the exchange-stiffness constant, the Dzyaloshinski-Moriya interaction, the mean magnetic anisotropy field, or the mean magnetostatic field due to jumps ΔM of the magnetization at internal interfaces. Besides the value of the applied magnetic field, it turns out to be the ratio of the magnetic anisotropy field H_p to ΔM , which determines the properties of the magnetic SANS cross section of bulk ferromagnets; specifically, the angular anisotropy on a two-dimensional detector (see figure below), the asymptotic power-law exponent, and the characteristic decay length of spin-misalignment correlations. Unpolarized and polarized neutron data on hard and soft magnetic nanocomposites will be discussed.

Keynote Speakers



(a)-(d) Contour plots of the normalized magnetic SANS cross section at applied magnetic fields as indicated ($\mathbf{k}_0 \perp \mathbf{H}_0$); $\mathbf{H}_0$ is horizontal in the detector plane). The change in angular anisotropy with increasing field that becomes visible in (a)-(d) reflects the competition between anisotropy-related and magnetostatic correlations. (e)-(h) Corresponding two-dimensional correlation functions $C(y,z)$ (for further details see Ref. [1]).

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Polymer-Nanoparticles Composites. Quo Vadis?

A.N. Ozerin, T.S. Kurkin, O.V. Lebedev, E.K. Golubev

Enikolopov Institute of Synthetic Polymer Materials, Moscow, Russia

ozerin@ispm.ru

Polymer composites (PC), which contain fillers dispersed in the polymeric matrix of a single-component or multiphase polymer blends continue to attract sustained attention from researchers and producers of polymer materials for the past several decades. Due to the simplicity and low cost of processing, features for customizing the set of properties for the final application, PC find a wide variety of practical applications.

Among the well-known methods of obtaining the PC (such as processing via solution, mixing in the melt, polymerization in situ, etc.), the technologies of melt mixing, using twin-screw extruders or injection molding are the most demanded by the modern industry of polymer processing. However, the necessity to reduce the volume content of the filler in the PC without losing the complex of the basic properties of the polymer matrix remains one of the most important scientific and technical challenges and is offered new and new types of the matrix polymers.

At the same time, the emerging new approach is constructing, based on the formation of the so-called segregated structures in the PC, which allows solving successfully the problem of low filler content in the composite. In the PC with a segregated structure, the dispersed filler particles are placed, with use of that or those approach, right on the border (interface) between the substructure units of the polymer matrix, instead of distribute them evenly throughout the volume of the polymer matrix.

In this paper, a comparative analysis is presented concerning new opportunities and unsolved problems in the field of development and design of a promising class of materials - polymer composites with a segregated structure. The potential application of SAXS and SANS methods is discussed in obtaining information about the spatial structure of such materials.

This paper discusses the prospects of using new types of composites with a segregated structure for a wide range of practical tasks and applications.

The investigation was performed at a financial support of the RFBR (project 14-03-01120) and the Program № 1 of the Presidium of RAS.

**Polarised proton spin density images tyrosyl radical locations
in bovine liver catalase**

O. Zimmer¹, H.M. Jouve², H.B. Stuhmann^{2,3}

¹ Institut Laue-Langevin, Grenoble, France,

² Institut de Biologie Structurale Jean-Pierre Ebel, Grenoble France

³ Helmholtz-Zentrum Geesthacht, Germany

heinrich.stuhmann@orange.fr

The A tyrosyl radical as part of the amino acid chain of bovine liver catalase supports dynamic proton spin polarisation (DNP). Finding the position of the tyrosyl radical within the macromolecule relies on the accumulation of proton polarisation close to it, which is readily observed by polarised neutron scattering [1,2]. The nuclear scattering amplitude due to the polarisation of protons with less than 10 Å distance from the tyrosyl radical is ten times larger than the amplitude of magnetic neutron scattering from an unpaired polarised electron of the same radical. The direction of DNP has been inverted each 5 s. The initial evolution of the intensity of polarised neutron scattering after each inversion was used to identify those tyrosines which have assumed a radical state. Three radical sites, all of them being close to the molecular centre and the heme, appear to be equally possible. Among these is tyr-369 the radical state of which had previously been proven by EPR [3].

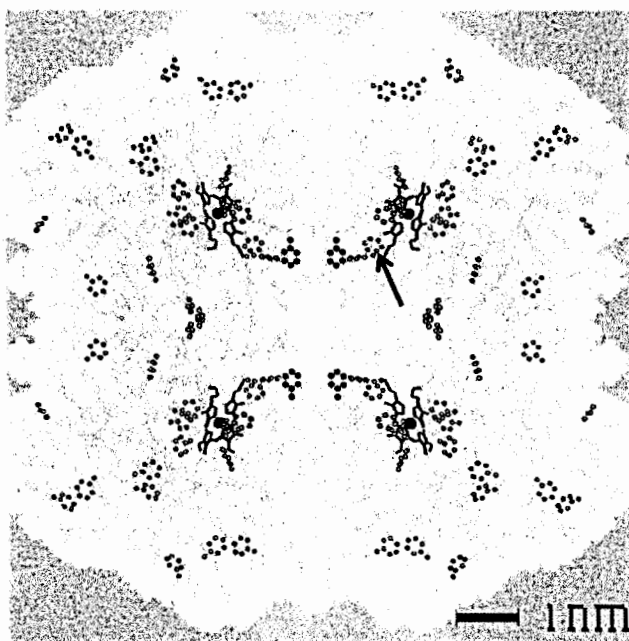


Fig. 1. The tetramer bovine liver catalase molecule with its tyrosines presented by their phenyl rings, most of them in orange colour. From neutron scattering it appears that one of the following tyrosines may have become a radical: tyr-324, tyr-357 and tyr-369. They are marked in blue colour. Tyr-136 (marked by an arrow) is another slightly less probable candidate. From EPR tyrosyl-369 is suggested (in dark blue). Tyr-357 is very close to the iron atom (●) of the porphyrin ring.

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The contribution of small angle scattering to the physics of liquid water

J. Teixeira

Lab. Léon Brillouin (CEA/CNRS), CEA-Saclay 91191 - Gif-sur-Yvette Cedex, France
jose.teixeira@cea.fr

Omnipresent and almost only liquid present on the Earth surface, water has unique properties which are not yet fully understood. Among the many unusual thermodynamic properties, the explanation of the density maximum at 277 K is a matter of debate. Because the anomalous behaviour is more pronounced at low temperature, many experiments were performed in the temperature region below the melting point, where the liquid state is metastable. However, nucleation of the solid phase prevents experiments below about 250 K, far above the glass transition temperature (135 K). Thus, a large domain of temperature of the order of 100 K remains totally unknown. As a consequence, many speculative models have been and are proposed, from the simple two-phase mixture of Roentgen till some recent simulations based on effective potentials describing the hydrogen bond molecular interaction.

Among several other scattering techniques, small angle scattering is the more direct way to evaluate the eventual existence of two phases. However, the weakness of the signal implies high accuracy in order to discriminate between contributions due density fluctuations from those due to concentration fluctuations. The first are associated to isothermal compressibility which anomalously decreases with decreasing temperature.

In this talk, a short review of the situation will be presented. Based on first principles of small angle scattering, the experimental results will be discussed and compared to a few theoretical approaches.

**Skippping between Portals:
Neutron analysis of membrane protein biogenesis**

N.R. Zaccai

Cambridge Institute for Medical Research, University of Cambridge, Cambridge, United Kingdom.
nrz201@cam.ac.uk

Contrast Variation Small Angle Neutron Scattering (SANS) has provided important insights into the biogenesis of Gram-negative bacteria. Their cell envelope consists of two membranes, the inner membrane and the outer membrane, that are separated by the periplasm. These membranes differ with respect to their lipid composition, but also in the structure of their integral membrane proteins. Importantly, the latter are synthesized in the cytoplasm, before being transported to their correct membrane.

For example, the chaperone protein Skp forms specific and stable complexes with outer membrane proteins while they are transported across the periplasm. X-ray and subsequent NMR data could not directly provide an explanation for the ability of Skp to bind a wide range of protein sizes. However, SANS experiments on Skp alone in solution and bound in two different complexes to outer membrane proteins, demonstrate that the helical tentacles of Skp bind their substrate in a clamp-like mechanism, which would allow direct interaction of the transported membrane protein with the outer membrane.

In the bacterial inner membrane, SecYEG, SecDF, YajC and YidC constitute the holo-translocon (HTL), with the capability for both protein secretion and membrane protein insertion. Contrast variation SANS revealed that the HTL complex contained a central lipid-containing pool, which conveys a compelling and unexpected mechanism for inner membrane protein insertion. In conjunction with electron microscopy analysis of the protein architecture of HTL, our results uncover a highly mobile complex capable of flexibly adapting its geometry and local environment to allow the folding and controlled release of an inserting membrane protein, reminiscent of the process of assisted folding for soluble proteins.

INVITED
SPEAKERS

Raman, CARS and SERS spectroscopy and microscopy: modern challenges and some applications

G.M. Arzumanyan

Joint Institute for Nuclear Research, Dubna, Russia

arzuman@jinr.ru

Optical microscopy is a unique technique among current imaging modalities in its ability to probe living specimens with subcellular resolution, enabling the visualization of morphological details in tissue and cells on the scale of a few hundred nanometers.

Raman spectroscopy and microscopy has become a mature analytical tool as a result of increased sensitivity and automation of the equipment over the past 20 to 30 years. In addition, the availability of multiple laser wavelengths whose choice is tailored to a particular application, as well as modern spectroscopic software coupled to 2D and 3D imaging, enhance the application of the technology.

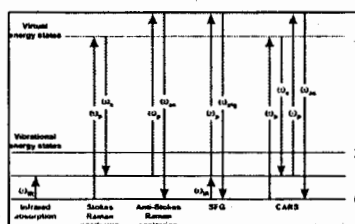


Fig. 1. Energy diagrams of IR and possible Raman processes

It's well known that the normal Raman scattering is weak – the cross-section of biological molecules is 10^{-30} - 10^{-26} cm² per molecule. That's why a number of methods were developed to increase the sensitivity of Raman probes. This presentation will cover the areas where Raman has made some impressive gains in biomedical sciences. These will include Raman and CARS (coherent antiStokes Raman scattering) imaging, including 3D one, of some biomolecules on the submicron level, surface-enhanced Raman spectroscopy (SERS) for signal enhancement targeted to specific bio-analytes, etc. Our first results on an application of Raman spectroscopy for disease diagnostics will be given as well.

Small-angle neutron scattering in structural research of detonation nanodiamonds

M.V. Avdeev

Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow Reg. Russia
avd@nf.jinr.ru

Detonation nanodiamonds (DND) are one of the products of the detonation of organic explosives with an imbalanced carbon-oxygen ratio biased towards the carbon content. They are diamond crystallites with a typical size of less than 10 nm, which makes them a very attractive material for nanotechnology. At present, of special interest is the combination of high specific surface and biocompatibility of DND. This is an important factor in the creation of nanocomposite materials for medical applications that use specific spectral properties of these nanoparticles. One of the main directions in the physical and chemical studies of DND concerns the purification and synthesis of their liquid suspensions in various solvents as a basis for the storage and subsequent chemical modification of nanoparticles. The availability of stable suspensions over a wide range of DND concentrations (up to 10 wt.%) makes it possible to apply [1-4] very effectively in structural research the method of small-angle neutron scattering (SANS) by using the contrast variation technique based on isotopic hydrogen-deuterium substitution in solvents. There are two fundamental aspects of the research presented: (I) structure of DND particles and their specific features at a nanoscale (characteristic size level of 10 nm); (II) cluster formation in the synthesis of DND and during their dispersion in liquid carriers (characteristic size level of 100 nm and higher).

It has been shown that DND particles reveal high size polydispersity (range from 2 to 10 nm) and exhibit a non-uniform inner structure. Thus, along with the predominant diamond component within the crystallites a graphite-like shell exists on the crystallite surface. This shell is also non-uniform and is characterized by a rather wide spatial diamond-graphite transition in terms of the radial distribution function of the scattering length density. It is responsible for the diffusive nature of the DND particle surface revealed in the scattering experiments as a specific deviation from the classical Porod law for particles with a smooth interface. To ensure a continuous diamond-graphite transition in DND, a characteristic diffusivity parameter is to be small, which can be observed in all the systems studied.

It has been shown that stable and reproducible fractal clusters with a wide size distribution from 10 to 100 nm and above (primary aggregation) are formed in liquid DND dispersions. The growth mechanism for the clusters characterized by a branched structure for both light and heavy

Invited Speakers

cluster fractions is unique irrespective of the dispergation procedure and polar liquid carrier. By its structural characteristics it is similar to the mechanism of diffusion limited aggregation (DLA). The branched structure of the primary clusters determines their overlap in the secondary aggregates.

A general theory of small-angle scattering on polydisperse particles with diffusive surface and their clusters has been developed and practically tested on DND suspensions. The approximation of small diffusivity has been considered to obtain simplified expressions for determining the parameters of the particle size distribution function based on experimental scattering curves. The behavior of different scattering invariants under contrast variation for this type of particles in solutions has been analyzed in detail. The effect of the mechanism of particle aggregation and growth in solution on the small-angle scattering curves has been studied.

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Neutron holography

L. Cser

Wigner Research Centre for Physics, Hungary
cser.laszlo@wigner.mta.hu

Neutron holography [1] achieving atomic resolution can be realized using either the internal source or the internal detector approach. The feasibility of both concepts has been proven in several experiments [2,3]. Recently [4], the inside detector technique was applied to an alloy where the concentration of holographic probe atoms is sufficiently low to consider them as impurities within a regular crystal lattice. In the present talk we demonstrate that atomic positions around such impurity atoms can be derived from a neutron hologram up to at least the fourth neighboring shell thereby attaining accuracy in the picometer range. In addition, it is shown that the observed local lattice distortion can be described by Friedel's model based on scattering of the conduction electrons by the impurity atom. This result suggests a promising new method for the direct observation of lattice distortions in the close vicinity of any local perturbation.

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Small-Angle Scattering of spheres: results for small volume fractions and special pair correlations

W. Gille

Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany
gille@physik.uni-halle.de

In Small-Angle Scattering (SAS) nanoparticles are investigated. The method is based on geometric models for the specific particle ensemble. On the one hand, such a model involves an assumption about the *particle shape* (assumption 1). On the other hand, the *spatial distribution* of the particles (assumption 2) influences the scattering pattern. Even restricting to spherical particles of varying diameter (assumption 1), there exist many approaches for describing the spatial positions of the particles. A field checked method, which enables the experimenter to introduce assumption 2, is the approach via a *pair correlation function* (PCF), see chapter 4 of the textbook [1].

The so-called pair correlation function of a *Dead Leaves model* (DLm), see [2,3] is operated with in the following. Contrary to many other approaches in this field, this function does not involve any approximation. For this DLm the volume fraction is fixed to $1/8$. However, it allows many modifications: It is interesting to decrease the sphere diameter x more and more, (i.e., up to zero), for a pair correlation corresponding to an initial diameter d . This leads to a dilution of the particle ensemble. Analytic expressions for the SAS correlation function(s) as depending on d and x result. The corresponding scattering patterns follow for a varying volume fraction up to zero.

An analysis of the scattering behavior shows: Coming from smaller to bigger scattering angles, for all diameters (including the limiting case of *scattering points*), the scattering intensity increases. A *typical maximum is reached*, followed by a more or less oscillating behavior.

Hence, there exist cases where a possible maximum in the SAS intensity is *not connected at all* with a relatively big volume fraction. The origin of the initial maximum of a SAS curve mainly should be traced back to the distribution of the distances between the centers of the particles. *Particle size and shape* are an effect of *second order* only.

A detailed investigation of the chord length distributions of diluted particle ensembles proves this rule. In the limiting case of a spatial point process, there does not exist a difference between *particle to particle chords* and *those distances*, which are *taken for the definition* of a pair correlation function.

Invited Speakers

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Studies on some iron oxide nanoparticles, nanocomposites and thin films for advanced applications

F. Iacomi

Alexandru Ioan Cuza University of Iasi, Romania
iacomi@uaic.ro

Iron oxide nanoparticles, nanocomposites and thin films are intensively studied due to their advanced applications in catalysis, medicine, and biotechnology. Ofen nanoparticles are isolated in zeolite materials or mineral clays or are included in polymer matrices in order to obtain certain properties [1-4].

In this paper the preparation conditions for iron oxide nanoparticles, $\text{Fe}_2\text{O}_3/\text{MCM-41}$ (0% Fe, 5% Fe, 10%Fe, 15%Fe - M, M5, M10, M15), $\text{Fe}_2\text{O}_3/\text{polymer+silica}$ nanocomposites (28% SiO_2 , 2% Fe_2O_3 , 4% Fe_2O_3 , 6% Fe_2O_3 - P1, P2, P3), hematite thin films and iron oxide/mineral clay nanocomposites (10.5% Fe -FCN, 18.0%Fe-FCIN), are presented together with the results obtained by studing their structural and functional properties.

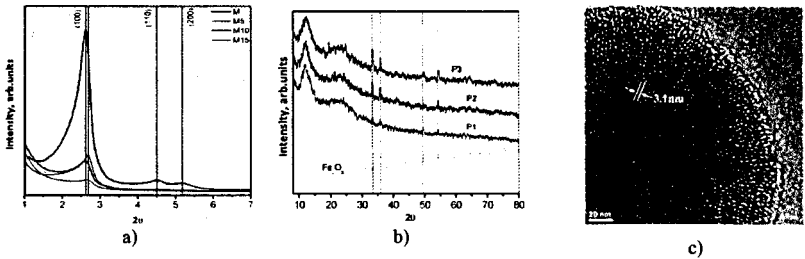


Fig.1. a) XRD patterns of $\text{Fe}_2\text{O}_3/\text{MCM-41}$ nanocomposites; b) XRD patterns of oxide/polymer+silica nanocomposites; c) HRTEM image of M sample (0%Fe).

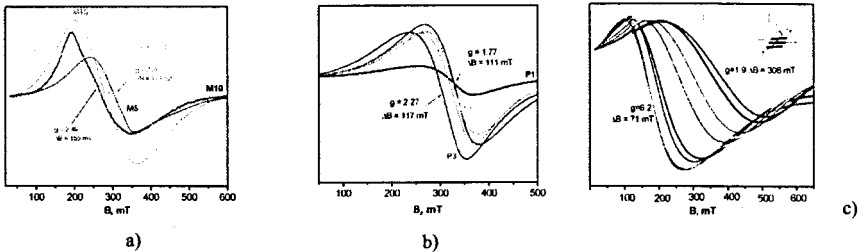


Fig.2. EPR spectra of iron in: a) MCM-41; b) iron oxide/polymer+silica nanocomposites; c) hematite thin films.

XRD, SEM, HRTEM, AFM and XPS investigations furnished informations related to the sample nanostructured character and chemical composition.

Room temperature EPR investigations evidenced that the sample magnetic anisotropy is dependent on the aggregation processes and that becomes more visible by increasing the pore sizes (MCM-41, mineral clay), the iron content, the silicon content (nanocomposites based on polymers), being higher in hematite thin films.

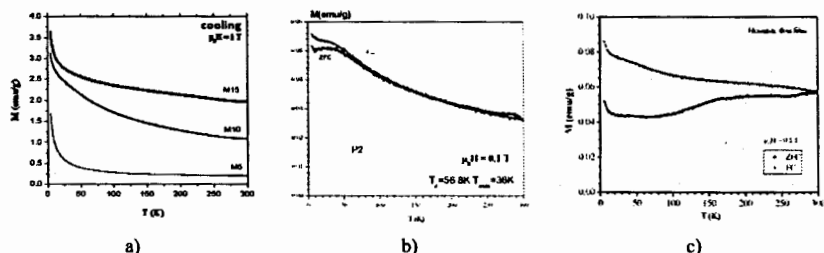


Fig.3. ZFC and FC magnetization curves for: a) iron oxide/polymer nanocomposites b) hematite thin film

Mössbauer spectra showed the iron oxide species: hematite and superparamagnetic iron oxide species for iron oxide/MCM-41 nanocomposites. ZFC and FC magnetization curves (Fig.3) enabled the evaluation of T_B (blocking temperature) and T_C (separation temperature) and to distinguish superparamagnetic from regular ferrimagnetic behavior.

EPR and magnetic investigations evidenced the importance of irradiation and annealing processes in controlling the iron oxide phases in iron oxide/mineral clay composites and the importance of covering magnetite nanoparticles with dextrane, polyethylene glycol or polyvinyl alcohol.

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Partially assembled nucleosome structures at atomic detail

G.N. Rychkov^{1,2}, A.V. Ilatovskiy^{1,3}, I. Nazarov⁴, A. Shvetsov^{1,5},
D. Lebedev¹, A. Konev¹, V. Isaev-Ivanov¹, A.V. Onufriev⁶

¹ Petersburg Nuclear Physics Institute, NRC "Kurchatov Institute", Gatchina, Russia, 188300

² Institute of Physics, Nanotechnology and Telecommunications, NRU Peter the Great St.Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg, Russia, 195251

³ Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, 9500 Gilman Dr, La Jolla, CA 92093, USA

⁴ Institute of Cytology, RAS, Tikhoretski Ave 4, Saint-Petersburg, Russia, 194064

⁵ Institute of Applied Mathematics and Mechanics, NRU Peter the Great St.Petersburg Polytechnic University, Polytechnicheskaya 29, Saint-Petersburg, Russia, 195251

⁶ Departments of Computer Science and Physics, Virginia Tech, Blacksburg, VA 24061, USA

isaev@omrb.pnpi.spb.ru

Evidence is now overwhelming that partially assembled nucleosome states (PANS) are as important as the canonical nucleosome for the understanding of how genome accessibility is regulated in cells. We use a combination of atomistic simulation and atomic force microscopy (AFM) to deliver, in atomic detail, structural models of three key PANS that occur on the nucleosome assembly/disassembly pathway: the hexasome (H2A·H2B)·(H3·H4)₂, the tetrasome (H3·H4)₂, and the disome (H3·H4). While the unbound DNA in these structures exhibits significant spatial fluctuations, regions of protected DNA maintain stable contacts with the remaining histones (~18 bp per histone), thus establishing the basis for understanding the role of PANS in DNA accessibility regulation. We suggest an alternative interpretation for a recent genome-wide study of DNA protection in active chromatin, leading to the conclusion that the three PANS are present in actively transcribing regions in substantial amounts. The presence of PANS may not only be a consequence, but also a prerequisite for fast transcription *in vivo*. We demonstrate how atomically detailed PANS can be used to gain novel qualitative and quantitative insights from *in-vitro* experiments: AFM, Förster resonance energy transfer, and small-angle X-ray scattering data obtained under conditions when PANS are expected to exist.

The Small-K Advanced Diffractometer SKADI, a multi-purpose SANS instrument at ESS for high impact science in soft matter and biological systems

J. Jestin¹, S. Désert¹, R. Hanslik², S. Jaksch², H. Frielinghaus²

¹ Laboratoire Léon Brillouin, CEA-CNRS, CEA Saclay, 91191 Gif/Yvette Cedex France

² Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, Garching, Germany
jacques.jestin@cea.fr

The pulsed source requires a time-of-flight analysis of the gathered neutrons at the detector. The optimal instrument length is found to be rather large, which allows for a polarizer and a versatile collimation. The polarizer allows for studying magnetic samples and incoherent background subtraction. The wide collimation will host VSANS option that increase the resolution of the instrument towards μm [2]. Two 1m^2 area detectors will cover a large solid angle simultaneously. The expected gains for this new instrument will lie in the range between 20 and 36, depending on the assessment criteria, when compared to up-to-date reactor based instruments. This will open new perspectives for fast kinetics, weakly scattering samples, and multi-dimensional contrast variation studies. The science cas and the high impact potential of the instrument will be illustrated through selected examples in soft matter and biological systems.

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The structural study of magnetoferritin and its complex systems by means of SAXS and SANS

**P. Kopčanský¹, L. Balejciková^{1,2}, M. Molčan¹, M. Timko¹, K. Siposová¹,
O. Strbak², M.V. Avdeev³, V.I. Petrenko^{3,4}, V.M. Garamus⁵,
L. Almasy⁶, K. Pospisková⁷, I. Safarik^{7,8}**

¹ Institute of Experimental Physics, SAS, Watsonova 47, 040 01 Kosice, Slovakia

² Institute of Measurement Science SAS, Dubravska cesta 9, 841 04 Bratislava 4, Slovakia

³ Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow region, Russia

⁴ Kyiv Taras Shevchenko National University, Volodymyrska Street 64, Kyiv, 01033 Ukraine

⁵ Helmholtz-Zentrum Geesthacht: Centre for Materials and Coastal Research, Max-Planck-Street 1, 21502 Geesthacht, Germany

⁶ Wigner Research Centre for Physics, HAS, H-1525 Budapest, POB 49, Hungary

⁷ Regional Centre of Advanced Technologies and Materials, Palacky University, Slechtitelu 11, 783 71 Olomouc, Czech Republic

⁸ Department of Nanobiotechnology, Institute of Nanobiology and Structural Biology of GCRC, Na Sadkach 7, 370 05 Ceske Budejovice, Czech Republic

kopc@saske.sk

Magnetoferritin (MFer) is biological complex composed of protein shell, apoferritin, and synthetically prepared magnetic iron oxides inside. Due to its unique properties (superparamagnetic behavior, nanoscale size and biological origin) it is believed to have various biomedical application (a contrast agent in radiology, a drug carrier in the targeted transport, or a standard in diagnostics of various diseases). Small Angle X-ray (SAXS) and Neutron (SANS) Scattering studies have shown partial shell destruction of MFer and increasing of polydispersity with the loading factor (LF: average number of iron atoms per one complex) growth [1,2]. Presence of magnetic nanoparticles in MFer could play an important role at observed ability to reduce the size and amount of lysozyme amyloid fibrils (LA), confirmed by SAXS and fluorescence measurements [3]. Such destroying effect of MFer on LA as model systems may help to understand pathology of neurodegenerative diseases. Moreover, MFer can be useful for potential applications as therapeutic agent against neurodegenerative diseases development. Next investigations using UV-VIS spectrophotometry have confirmed peroxidase-like activity of MFer [4] what allows its potential use in nanocatalytic chemistry or for colored visualization of tumor tissues via MFer interactions with receptors highly expressed on cancer cells. Preliminary calorimetric measurements have shown the increase in temperature during exposition of MFer in AC magnetic field during magnetic hyperthermia tests. Our extensive studies and many results suggest that MFer complex behavior is related mainly to the unique properties of magnetic nanoparticles associated with its reactive surface and nano-size mainly. Presence of magnetic nanoparticles in MFer affects also the contrast at Magnetic Resonance Imaging (MRI). MRI

method could be useful for diagnosis and identification of illness associated with magnetic nanoparticles formation in damaged ferritin at neurodegenerative or cancer diseases, while MFer would be suitable standard or contrast agent.

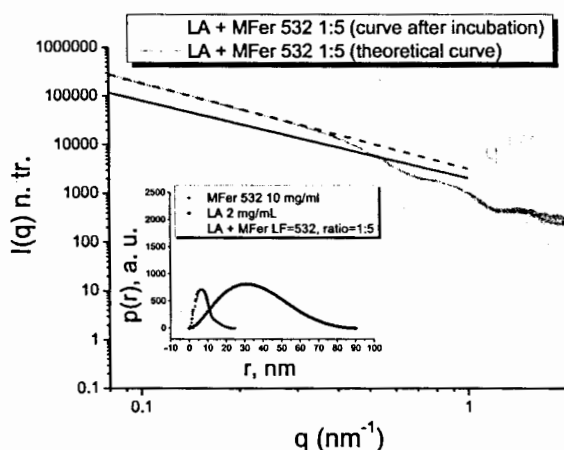


Fig. 1. A) Theoretical (grey) and experimental (pink) averaged SAXS curves of lysozyme amyloid fibrils (LA) after interference with MFer with loading factor 532 (LA : MFer 532 = 1:5). The initial parts of curves were modeled with the power-law, $q^{-1.77}$ and $q^{-1.6}$ corresponds to a mass fractal with dimension $D_s = 1.77$ and 1.6. B) PDD functions of LA with MFer 532 solution (pink) compare to curves for LA (black) and MFer (red) [3].

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Condensed Matter Research at Frank Laboratory of Neutron Physics

N. Kučerka

Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna - Moscow region, Russia
Faculty of Pharmacy, Comenius University in Bratislava, Bratislava, Slovakia
kucerka@nf.jinr.ru, norbert.kucerka@fpharm.uniba.sk

Each Laboratory has its own prehistory and destiny. The establishment of Frank Laboratory of Neutron Physics dates back 60 years, and is connected closely to the first and only pulsed reactor in the world. The economic advantages of IBR-2 reactor allow to run the facility for many past and future years. The idea behind this unique machine, its history, and present will be discussed. Most importantly, the examples of possible scientific investigations will be presented from a wide range of condensed matter research, not forgetting the field of soft matter and biomembranes.

Small angle neutron and X-ray studies of carbon structures with metal atoms

V.T. Lebedev

Petersburg Nuclear Physics Institute, NRC Kurchatov Institute, 188300 Gatchina, Leningrad distr., Russia
 vlebedev@pnpi.spb.ru

A review of recent activity at PNPI in the studies of carbon structures with metal atoms has been presented concerning fundamental aspects and applications in biomedicine and nuclear technologies. Self-assembly of water-soluble derivatives of endofullerenes with rare earth elements in solutions is discussed in terms of fractal models as dependent on concentration, pH and the temperature of medium [1,2]. The peculiarities of structural organization of aqueous solutions of first prepared endofullerenols with iron atoms are considered as compared to the properties of ensembles of reference objects $Gd@C_{82}(OH)_X$ ($X=30-40$) which are the effective agents for Magneto-Resonance Imaging (MRI) (Fig.1,2).

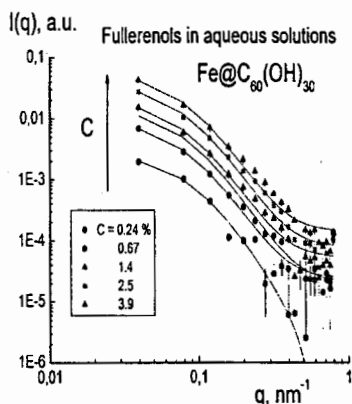


Fig.1. SANS: $Fe@C_{60}(OH)_X$ aqueous solutions ($20^\circ C$), contents $C = 0.24-3.9$ wt.%. Fitting functions $I(q) = I_0[1 + (qR_c)^2]^{-2}$ are dependent on forward scattering intensity $I_0(C)$ and clusters' correlation radius $R_c(C)$.

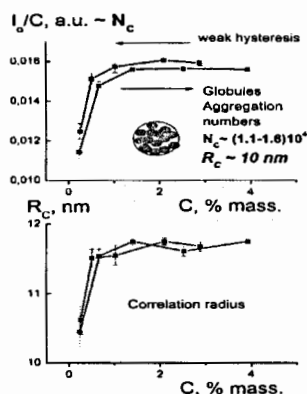


Fig.2. Forward intensity $I_0(C)/C$ normalized to molecular concentration and globular clusters' correlation radius $R_c(C)$ vs. fullerenols' content. The values $I_0(C)/C \sim N_c$ are proportional to the concentration of clusters N_c .

New molecular objects $Fe@C_{60}(OH)_X$ synthesized for this purpose demonstrate a globular aggregation into massive supramolecular structures (number of molecules $N_c \sim 10^4$, correlation radius $R_c \sim 10$ nm) being stable in solutions in the range of concentrations $C \sim 0.5-4$ % wt. This assembly improves fullerenols' functional properties (MRI contrast efficiency).

On the other hand, alternative types of carbon structures being ultra porous matrices with metal atoms captured inside small cells have been analyzed by SANS and SAXS [3]. These methods have been applied to the study of pyrolysates of diphthalocyanines containing various elements (Y, La, Ce, Nd, Tb). Such developments in the synthesis of composites have provided the encapsulation of heavy elements and nuclides to prevent their pollution outside the matrices even at high temperatures during long time storage. A formation of porous carbon structures have been discovered as dependent on annealing temperature, atomic number and mass of basic elements. Low-temperature process (800°C) created rare structures with a small amounts of atoms while above (1000-1600°C) it was detected the integration of carbons into globules (size ~ 1 nm, number of atoms $m \geq 100$) (Fig.3).

Small-sized carbon globules create branched fractal structures at the scale of few tens of nanometer which are integrated into massive structures inducing intense scattering. Finally it was found a similarity of such matrices, multilayered carbon “onions” and volcanic material (shungit) that indicates a universal mechanism governing self-assembly of carbon atoms at high temperatures.

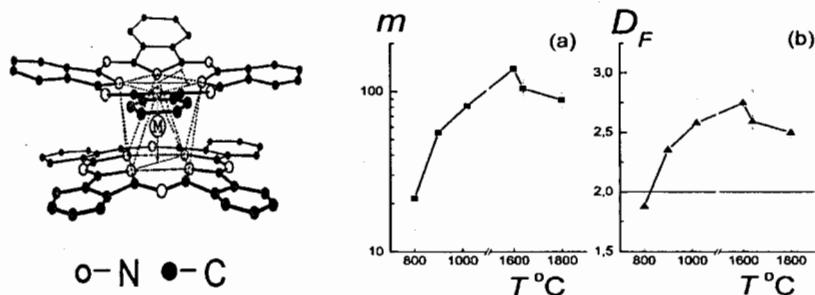


Fig.3. Diphthalocyanine (left). Aggregation number $m(T)$ (a) and fractal dimension $D_F(T)$ (b) of carbon globular structures obtained from La-diphthalocyanine by pyrolysis at the temperatures 800-1800°C (right).

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Nuclear-magnetic interference effects in small-angle scattering of polarized neutrons

Runov V.V.

Petersburg Nuclear Physics Institute, NRC "Kurchatov Institute", Gatchina, Russia
runov@pnpi.spb.ru

Scattering of polarized neutrons has a very important advantage in comparison with the scattering of non-polarized ones, as in this case it is possible to allocate the part determined by the magnetic nuclear interference scattering, i.e. to measure the product of the nuclear scattering amplitude (A) on magnetic amplitude (B), (AB). As shown in this report, the allocation in SAPNS (Small-Angle Scattering of Polarized Neutrons) method is highly efficient for the solution of some specific problems. **This efficiency is based on the possibility to study nuclear-magnetic scattering in contrast to the general, much more powerful magnetic or nuclear (or both) small-angle scattering. Performing this task is like looking for a needle in a haystack. Nevertheless, it can be solved due to the mutual magnetic-nuclear contrast enhancement of scattering.** The interference scattering $\Delta(q)$ is measured as the difference in the intensity of scattering with polarized neutrons up/down the magnetic field applied to the sample, that is, $\Delta(q) = I^+(q) - I^-(q) \approx P(AB)$, where P is the neutron polarization through the sample. Thus, the effect of the interference is measured at zero background in absence of interference. Examples of studies magnetic correlation are shown in the report: 1) 3-d impurities in nonmagnetic matrix [1]; 2) the evolution of magnetic-nuclear contrasting fraction in magnetic alloy under treating [2]; 3) ferromagnetic nanoparticles in the polymer, and others. The results presented in this report were obtained at PNPI (WWR-M) after the upgrade of the small – angle installation of polarized neutrons "Vector".

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Lipid based drug delivery systems: Kinetics by SANS

D. Uhríková¹, J. Teixeira², L. Hubčík¹, A. Búcsi¹,
T. Kondela¹, T.N. Murugova^{3,4}, O.I. Ivankov^{3,4,5}

¹ Faculty of Pharmacy, Comenius University in Bratislava, Bratislava, Slovakia

² Laboratoire Léon Brillouin CEA Saclay, France

³ Frank Laboratory of Neutron Physics, Dubna, Russia

⁴ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁵ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

uhrikova@fpharm.uniba.sk

One of the main challenges in pharmaceutical therapy are targeted drugs delivery systems. Significant efforts have converged in the past years towards the design and development of on-demand delivery systems based on functionalized lipidic liquid crystalline matrices. Lyotropic liquid-crystalline phases formed by the swelling of certain lipids (lipid/surfactant mixtures) when exposed to aqueous environments comprise: one-dimensional lamellar phase known as liposomes in excess water; two dimensional columnar hexagonal phases (hexosomes); and three dimensional cubic phases of symmetries characterized by space groups (cubosomes). In addition to polymorphic behaviour of the drug delivery system both processes, the drug packing and its release are important.

We will demonstrate several examples of polymorphic behaviour and kinetics of drug packing /release for nucleic acids delivery vectors. Either a condensed lamellar or inverted hexagonal phase was formed due to DNA interaction with phospholipids in presence of divalent metal cations. Divalent metal cations mediate DNA interaction with phospholipid bilayer forming supramolecular aggregates able to transfer DNA into a cell. A mixture of monoolein and pH responsive surfactant N,N-dimethyldodecylamine-N-oxide in excess of water forms a cubic phase of Pn3m symmetry. The lipid/surfactant molar ratio modulates lattice parameter of the cubic phase. Both techniques small angle X-ray diffraction (SAXD) and small angle neutron scattering (SANS) were employed to examine the structure of delivery vectors, while kinetics of the vector formation (or disintegration) was followed by SANS. Kinetic SANS experiments were performed at YuMO spectrometer.

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Nanostructured titanium based materials synthesized by Thermionic Vacuum Arc (TVA) method for industrial applications

R. Vladoiu, A. Mandes, V. Dinca-Balan, G. Prodan

Ovidius University, Constanta, Romania

rvladoiu@univ-ovidius.ro

The knowledge of interrelations between nanoscale deformation and strength mechanisms and the service properties of the materials is the way to find the reserves of optimization, improve the fabrication technology or predict the service properties of nanomaterials. This paper will highlight some of the most important developments in the present state of the art in scientific research and industrial practices that involve titanium (Ti) based films in different combination prepared by Thermionic Vacuum Arc (TVA) method (Ti-Mg, Ti-Ag and Ti-Cr).

The morphologies and compositions of the coated surfaces by TVA were examined by scanning electron microscopy (SEM), atomic force microscopy (AFM), transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDS) in order to identify the wear mechanism. Corrosion, debris adhesion, and oxidation were found to be the dominant wear processes. When analyzing the mechanical properties of nanostructured metals, one should take into account the peculiar mechanisms of deformation, the role of the grain boundary phase, the mechanisms of grain boundary sliding and diffusional mass transfer. This is why one of the main reason of our study is concerning with the grain size distribution.

The Ti-Mg thin film exhibit an amorphous structure, with polycrystalline grain mainly being Mg hexagonal phase and small amount of hexagonal Ti. Grain mean size was estimated to be ~120nm by statistical analysis of measured Feret diameter of projected area of grain. The phases were tested by mean of Cohen method applied to electron diffraction results. No oxide (MgO, TiO₂) lines could be identified from electron diffraction. Debye-Scherrer dimension, estimated from electron diffraction profile is ~4 nm. The analysis of amorphous part from diffraction profile show different coordination number for Mg and Ti atoms.

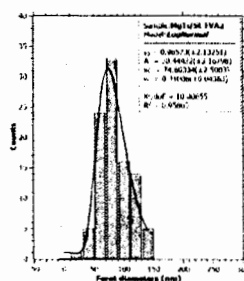
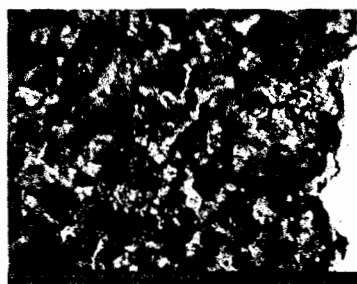


Fig 1. Grain size distribution of the Ti-Mg thin film deposited on glass

Sample	Cristalline structure	Network parameters [1]	relative errors (%) [2]
		Cohen	Cohen
MgTi/Si	Hexagonal (Mg, Ti)	Mg ($a_0=3,1874 \text{ \AA}$, $c_0=5,0595 \text{ \AA}$)	Mg (0,69%, 2,9%)
		Ti ($a_0=3,0002 \text{ \AA}$, $c_0=4,5561 \text{ \AA}$)	Ti (1,70%, 2,77%)
MgTi/Gl	Hexagonal (Mg, Ti)	Mg ($a_0=3,285 \text{ \AA}$, $c_0=5,306 \text{ \AA}$)	Mg (2,35%, 1,84%)
		Ti ($a_0=2,878 \text{ \AA}$, $c_0=4,486 \text{ \AA}$)	Ti (2,41%, 4,25%)

In case of Ti-Ag deposited on silicon the structure is an amorphous matrix, with partial cristallized region.

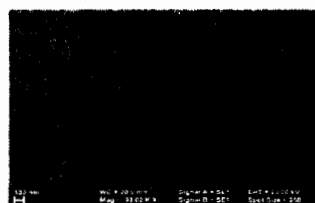


Fig. 2. SEM image on Ti-Ag/Si sample deposited by TVA method

Ti-Ag/Gl sample has polycrystalline structure with 300-500 grains where cubic Ag is embedded in Titanium matrix. Most important developments of the behavior of the shafts, gears, impellers as part of gearboxes, turbines and mobile irrigation machines coated with different nanocomposite in different environment are envisaged in the future work.

Acknowledgements

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Size and Structure Characterisation of Nanoparticles by Small-Angle Scattering: Uniqueness, Reliability, Methods

V.V. Volkov

Shubnikov Institute of Crystallography of Federal Scientific Research Centre "Crystallography and Photonics"
of Russian Academy of Sciences
yvo@ns.crys.ras.ru

Small-angle X-ray (SAXS) and neutron (SANS) scattering is widely used to study the structure of matter at a supramolecular level up to several hundred nanometers. This range corresponds to the size of the structural components of all types of nanosystems. The most important feature of small-angle scattering (SAS) is the possibility of analysis of the structure of disordered systems, and often its use is the only way to obtain information about the structure of the samples with a random arrangement of nanoscale inhomogeneities. Sometimes, particularly important is the fact that samples can be studied by SAS in their natural state, without any specific preparation: liquids, gels, polymeric systems, disperse powders, biomolecules in solution, etc. [1].

For **polydisperse** systems of nanoparticles (in general case - the inhomogeneities) the most often parameters that are determined from SAS data are size distributions with a priori given forms of particles (spheres, cylinders, ellipsoids, etc.). Two basic approaches are used for calculating the distributions - determination of a smooth distribution function by a regularization method [2] and modeling of superposition of distribution functions given in an analytical form [3]. The scattering data from **monodisperse** system (the most typical example - solutions of protein molecules) allow one to relatively reliably determine the so-called invariants - maximum size, radius of gyration, volume, (surface area), and a distance distribution function. After evaluation of the invariants a number of programs [4-6] may be applied to define the shape of the particles with a resolution of 1/3 of 1/5 of the maximum size (taking into account the additional information - and at a higher resolution).

Such inverse problems, both for polydisperse and monodisperse systems, mathematically are usually ill-conditioned, which requires both the development of stable algorithms for finding a solution, and the use of practical experience. The presentation addresses many of the practical and theoretical aspects of the interpretation of small-angle X-ray and neutron scattering data.

In particular, the algorithm for search of size distributions, which is based on the building a linear combination of partial analytical functions [3] is very sensitive to the choice of angular spacing. To reduce the instability of the results, it may be modified in several respects.

Invited Speakers

1) The stability may be improved by introducing nonequidistant angular grid to calculate the R-factor. 2) A more efficient algorithm for finding the minimum of the target function may be used like NL2SOL (Levenberg-Marquardt algorithm, enhanced by approximation of Hessian matrix using the variable metric scheme). 3) A secondary search for a solution may be applied based on the minimization of the residuals weighted by the inverse function of the relative systematic residuals which are calculated from statistical analysis of the residuals obtained after the first iteration of the search.

Restoration of 3-dimensional shape of the particles from SAS is not only ill-posed, but also ambiguous problem. Both of these factors lead to the spread of solutions, which also depends on the parameters of the models (in particular, bead size) and angular data range. The spread of the solutions can be reduced by modification of the search scheme used. The basic idea consists in a periodic variation of the relative magnitudes of penalty terms of the objective function.

Finally, some general quality criteria for solving inverse problems are considered, based on the calculation of the relative systematic error in the difference between the experimental and model scattering data.

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CONTRIBUTED TALKS

Iron oxide nanostructures – investigation of microstructural and magnetic properties

E. Puscasu¹, L. Sacarescu², N. Lupu³, M. Grigoras³, M. Balasoiu^{4,5}, D. Creanga¹

¹ Faculty of Physics, Alexandru Ioan Cuza University, Iași, Romania

² P. Poni Institute of Macromolecular Chemistry, Iași, Romania

³ National Institute of Research and Development for Technical Physics, Iași, Romania

⁴ Joint Institute for Nuclear Research, Dubna, Moscow Region, Russian Federation 141980

⁵ Horia Hulubei Institute of Physics and Nuclear Engineering, Bucharest, Romania

e-mail of corresponding author: dorina.creanga@gmail.com

Iron oxide nanoparticles (MNPs) prepared by chemical co-precipitation were dispersed in aqueous suspension by coating with oleate double shell [1-2]. Further the sol-gel procedure was applied for MNP silanization [3]. Good crystallinity and granularity as well as dominant superparamagnetic properties of both oleate/MNPs and silica/oleate/MNPs were revealed by X-ray diffractometry, Transmission and Scanning Electron Microscopy, Small Angle X-ray Scattering, Energy Dispersing X-ray Analysis and Vibrating Sample Magnetometry.

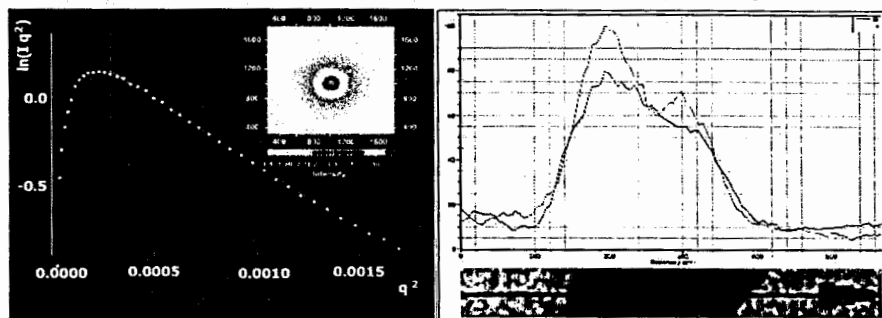


Fig. 1. a) left- SAXS investigation result of MNPs; b)right-EDX scanning of silica coated MNPs

Oleate/iron oxide MNPs bioeffects were tested on animal cell cultures revealing cell viability decreasing and DNA injuries [2] while silica/oleate/iron oxide nanocomposites are going to be functionalized with biomolecules for medical applications.

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Small angle scattering instrument YuMO

O.I. Ivankov^{1,2,3}, D.V. Soloviev^{1,2,3}, A.V. Rogachev^{1,2}, Yu.S. Kovalev^{1,2}, A.P. Sirotnin¹,
A.S. Kirilov¹, T.B. Petukhova¹, A.G. Soloviev¹, T.M. Solovjeva^{1,2}, A.I. Kuklin^{1,2}

¹ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

ivankov@jinr.ru, dimkaupml@gmail.com, kuklin@nf.jinr.ru

The current status of YuMO spectrometer with changes realised is presented. Main feature of instrument, namely: two detector system [1,2]; thermal spectrum (due to comb-like water moderator) of neutron wavelength; good collimation; Vn-standard in front of each detector; direct beam detector in end of beam-line; automatization of almost of all part etc. are shown. Main devices for sample environment on 4-th beam-line of IBR-2M reactor are described [3]. The short review of realized at spectrometers investigations in field of biology, polymers, material science and physical chemistry are given. It was shown that spectrometer has the world level of submolecular structure investigations. Some papers prepared by analyzing of data obtaining at YuMO spectrometer are discussed. The prospect and possible way of spectrometer for future are discussed also.

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Fine structure and performance of perfluorinated proton conducting membrane systems

Yu.V. Kulvelis¹, S.S. Ivanchev², O.N. Primachenko², V.T. Lebedev¹, A.I. Kuklin³

¹ B.P. Konstantinov Petersburg Nuclear Physics Institute, National Research Centre «Kurchatov Institute», Gatchina, Russia

² St. Petersburg Department of Boreskov Institute of Catalysis, Siberian branch of Russian Academy of Sciences, St. Petersburg, Russia

³ Joint Institute for Nuclear Research, Dubna, Russia

kulvelis@pnpi.spb.ru

The recent development of hydrogen power has initiated the studies of perfluorinated membranes based on copolymers with shortened side chain length (SSC), while earlier the attention was focused mainly on long side chain (LSC) membranes. These are perspective materials to be used as membranes in hydrogen fuel cells. SSC membranes have advantages over LSC, performing higher proton conducting properties and working at higher temperatures, allowing use of less pure hydrogen as a fuel. SSC membranes will increase the efficiency of hydrogen fuel cells and expand their application area. Fig. 1 demonstrates standard way of synthesis and resulting chemical structures of LSC and SSC perfluorinated polymers.

Small-angle neutron scattering (SANS) on SSC membranes has discovered their fine structure peculiarities. The general structure elements for SSC membranes are similar to those observed for LSC membranes – regularly arranged cylindrical channels forming ordered structure. The difference of SSC and LSC membranes appears in thinner channels for SSC samples, along with larger proton conductivity, closed to each other neighbour channels and different geometry of channels, varying significantly from slightly curved to branched. According to SANS experiments of LSC and SSC membranes prepared by different methods we note that the larger channel distribution density, lower thickness and larger dynamicity of channels when moistening are accompanied by larger values of proton conductivity [1-2]. Structure peculiarities of SSC membranes modified with orientation hood, leading to additional ordering and rising of proton conductivity, were also studied.

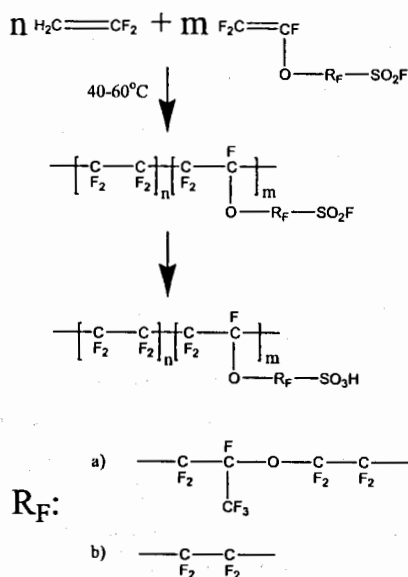


Fig. 1. Synthesis route for LSC (a) and SSC (b) perfluorinated polymers. n and m varies membrane composition

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Application masking liquid technique for SAXS study of nanocomposites

Yu.V. Larichev^{1,2}

¹ Borekov Institute of Catalysis, Siberian Branch of Russian Academy of Sciences, Prospekt Akademika Lavrentieva 5, Novosibirsk, 630090, Russia

² Novosibirsk State University, Pirogova Street 2, Novosibirsk, 630090, Russia
ylarichev@gmail.com

Natural bio-resources (rice husk, peat, sapropel and other) have a big perspective as a source for preparation different types of low-cost carbon and carbon-mineral adsorbents and functional materials. Typical problem for wide application of these materials in industry it is unsatisfactory reproducibility of main properties due to preparation these materials. The base reasons of this problem are complex composition of natural material, amorphous structure and respectively poor information about particle sizes and shapes of mineral parts of materials. These data are needed for understanding process of formation porous structure due to calcination and activation such bio-resources. Removing of mineral part (totally or partially) could noticeably increase specific surface of these materials. Depends on the mineral part content and their particle shape and sizes in material it is possibly to consider carbon porous structure with inorganic inclusion or vice versa porous mineral matrix covered by carbon film. Nevertheless information about inorganic particle sizes and their shapes in initial bio-materials practically is absent. One of the methods is suitable for obtaining data about particle sizes in bio-materials is small angle X-ray scattering with using special masking liquid for masking parasitic scattering signal from organic part of matrix [1]. In this work will discussed possibility this technique for bio-materials analysis. Moreover will be reported results of analysis of mineral components (particle size distribution and particle shapes) in rice husk, peat, sapropel and brown coal.

The author is grateful to P.M. Yeletsky, O.I. Krivonos and E.V. Maltseva for samples provision. This work was supported by the Russian Science Foundation (grant no. 14-23-00037).

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Effect of molecular crowding modulating agents on chromatin structure revealed by SANS

D.V. Lebedev, R.A. Pantina, M.V. Filatov, V.V. Isaev-Ivanov

Petersburg Nuclear Physics Institute, NRC "Kurchatov Institute", Gatchina, Russia
dtry@omrb.pnpi.spb.ru

Interphase chromatin exhibits large variations in density of packing, from highly structured dense heterochromatin to the transcribed regions of euchromatin which are characterized by lower density and high nucleosome dynamics. Evidence for the fractal organization of genetic material come from a number of studies [1]. There has been a clear indication that the nucleosome structure and small-scale in intact nuclei of abnormally proliferating cells differs from that of both non-proliferating (chicken erythrocyte) and normally proliferating cells [2]. Direct modeling of the fractal organization of intact unmodified nucleosomes in the broad range of scales have shown that the model can describe the experimental data in fractal regime but fails on the small scales, especially for fast-proliferating cancer cell lines [3].

Small-angle neutron scattering experiment on isolated nuclei of chicken erythrocytes and C6 rat glioma cells revealed profound changes in both small- and large-scale chromatin structure following treatment by polyethyleneglycole with the MW between 3000 and 20000. PEG treatment have irreversibly increased the scattering near $0.06 \text{ \AA}^{-1}$ that corresponds to the average size of the nucleosome (11 – 13 nm). At the same time, the fractal regimes at the lower q have also changed to surface fractal dimensions between 0.004 and $0.02 \text{ \AA}^{-1}$. Effect of PEG of different molecular weight on the scattering in the fractal region had differed dramatically depending on the molecular weight of the polymer. The strong dependence of the scattering on its molecular weight could be connected to the different effect of PEG-3000 and PEG-20000 on macromolecular crowding conditions inside the nucleus. A small but noticeable effect of urea treatment on the chromatin structure observed also suggests that macromolecular crowding could play a role in chromatin self-organization.

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Cylindrical flexible micelles of ionic surfactant produced by nonorganic salts

V.S. Molchanov, A.L. Kvyatkovsky, O.E. Philippova

Physics Department, Lomonosov Moscow State University, Moscow, Russia
molchan@polly.phys.msu.ru

Wormlike micelles of surfactant molecules are giant polymer-like chains that create a transient network in an aqueous medium. The system exhibits high viscoelastic properties which fully recovery through self-assembly after applying a high deformation, a stress or pressure as a result of noncovalent bounds between molecules in the chain. The ionic surfactant molecules with long tail (hydrophobic part) at the presence of a salt usually aggregate into enormously long flexible cylindrical micelles so-called wormlike micelles. The viscoelastic properties are highly sensitive to many factors, for example, concentration of a salt, presence of hydrocarbons or temperature due to shape and length variation. Highly responsive viscoelastic properties which would be recovered and outstanding transformation of the micelles are attracted attention of scientists and industry companies. So, the surfactant solutions are often used in industry at thickening agents in paints, cosmetics, food. In oilfield industry the wormlike micelles solutions are applied as main component of fracturing fluids in oil recovery. Recent publications have demonstrated the network wormlike micelles as matrix in smart magnetorheological fluids and open new field for applications and supporting investigations. From scientific point of view the wormlike micelles are used as large hydrophobic containers for synthesizes, as model of polyelectrolyte solutions. Nevertheless, amount of the publications devoted to the wormlike micelles growth and transformation remains high in spite of more than 20 years active researches in the field.

In the present work the viscoelastic properties of the aqueous solutions of the cationic surfactant erucyl bis(hydroxyethyl)metilammonium chloride (EHAC) with inorganic mono- and multivalent salts are observed. The investigation allows us to describe the coions and the counterions effects on the micellar growth and branching.

Rheological properties of long tailed surfactant aqueous solutions were examined as function of multivalence nonorganic salts concentration. SANS data, Cryo-TEM pictures and analysis of rheological curves indicate growth of linear wormlike micelles and branching. Increase of density of packing of surfactant molecules in wormlike micelles was obtained with SANS experiments upon salt addition. It was obtained that multivalence salt initiates dilute semidilute transition of the micelles at lower concentration. The effect was neglected when

rheological properties curves was plotted as function of the counterions content. It was obtained that maximum values of the zero-shear viscosity, elastic modulus and relaxation time depend on coions type. Well defined three regions of zero-shear viscosity and relaxation time were observed upon salts content. These regions were correlated to growth of the length and branching formation due to counterions and coions influence. Dissociation of counterions and condensation of coions with increasing the salts content and density of the network was suggested as reason for the observed phenomena.

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Dielectric Universalities and Charge Transport in Bacterial Filaments: Structural Data from SANS

K.A. Motovilov¹, A.A. Pronin², E.S. Zhukova^{1,2,3}, Z.V. Gagkaeva¹, V.I. Torgashev⁴, M. Savinov⁵, V. Grinenko⁶, M.A. Belyanchikov^{1,2}, A.K. Grebenko¹, M.A. Letarova⁷, K.V. Sidoruk⁸, T.N. Murugova^{1,9}, O.I. Ivankov^{1,9,10}, M. Dressel³, B.P. Gorshunov^{1,2,3}

¹ Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Moscow Region, Russia

² A.M. Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, 119991, Russia

³ 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, 70550, Germany

⁴ Faculty of Physics, Southern Federal University, Rostov-on-Don, 344090 Russia

⁵ Institute of Physics, ASCR, Prague 8, 18221, Czech Republic

⁶ Leibniz Institute for Solid State and Materials Research Dresden, Dresden, PF 27 01 16, D-01171, Germany

⁷ Winogradsky Institute of Microbiology, Russian Academy of Sciences, Moscow

⁸ Scientific Center of Russian Federation Research Institute for Genetics and Selection of Industrial Microorganisms, Moscow, 117545, Russia

⁹ Joint Institute for Nuclear Research, Laboratory of Neutron Physics, Dubna, Russia

¹⁰ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine
oven24@gmail.com

Bacterial filaments represent an extremely wide class of objects related with various functions: attachment of bacteria to the solid surface, DNA exchange between cells, motion of bacterial cell within medium, electron transfer from cell to the solid substrate etc. Clear understanding of composition and structural organization of the filaments remains to be a challenge since the studies of these objects meet a lot of severities which arise from the problems of growth, isolation and purification of filaments. One of the most interesting properties and functions of the known bacterial filaments is their ability to transfer electrons on rather long distances (up to dozens of microns). The most intensive investigations of charge transfer in bacterial filaments were performed on bacterial strains *Shewanella oneidensis* MR-1¹⁻⁴ and *Geobacter sulfurreducens*⁵⁻⁹. It was demonstrated that in the case of *S.oneidensis* the efficiency of electron transfer depends on expression of various multiheme cytochromes² which, as it seems to be, form periodic structures within filaments⁴. It is still not clear whether the conductive filaments of *S.oneidensis* are pure protein structures or they are appendages of outer cell membrane containing some lipids and peptidoglycans⁴. In case of *G. sulfurreducens* conductive filaments are the pili of IVth type^{5,10}. They have more simple structure than the filaments of *S.oneidensis* MR-1 and contain pilin protein conjugated with some cytochromes exposed to environment¹⁰. The mechanism of charge transfer within conductive bacterial filaments is the matter of intensive debates. Several groups argue that they observe so-called organometallic conductivity in filaments of *G.sulfurreducens* with classic dependencies of conductivity from temperature and pH⁶⁻⁹. Others say that it is almost impossible to form close stacking of aromatic

amino acids within known pilins¹¹. The absence of high resolution structural data leads to debates based only upon indirect measurements and estimations. In the case of *S. oneidensis* MR-1 there is general agreement that electron transfer in filaments is based on hopping mechanism within multiheme cytochromes^{2,12,13}. At the same time there is no any experimental data or theoretical insights on possible role of ion transfer along conductive filaments both inside and outside them. Ionic charge transfer should occur in natural aqueous environment of bacteria and may play key role in the whole process of conjugated electron and proton transfer by filament. Importance of water channel inside filaments for effective ion transfer within them is obvious. By means of SANS we clarified the presence of water channel inside filaments and existence of lipid components within *Shewanella oneidensis* MR-1 filament's wall.

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Study of visual pigment rhodopsin supramolecular organization in photoreceptor membrane by SAXS and SANS

M.A. Ostrovsky^{1,2,3}, T.B. Feldman^{1,2,3}, O.I. Ivankov^{4,5,6}, T.N. Murugova^{4,5},
A.I. Kuklin^{4,5}, M.A. Yakovleva², V.I. Gordeliy^{5,7,8}, A.V. Belushkin⁴

¹ Department of Molecular Physiology, Biological Faculty Lomonosov Moscow State University, Moscow, Russia

² Emanuel Institute of Biochemical Physics Russian Academy of Sciences, Moscow, Russia

³ Laboratory of Radiation Biology, Joint Institute for Nuclear Research, Dubna, Russia

⁴ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

⁵ Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia

⁶ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁷ Institut de Biologie Structurale, Grenoble, France

⁸ Research Center Juelich, Juelich, Germany

The visual pigment rhodopsin is a prototypical member of a large G-protein-coupled receptor (GPCR) family, which plays a key role in all regulatory processes of living organisms [1]. Like many other membrane receptors, GPCRs are known to form dimers and high-order oligomers in membranes. However, the supramolecular organization of rhodopsin in photoreceptor membranes is discussed. Atomic force microscopy images of the native rod outer segment disk membranes showing the rows of rhodopsin dimers provide a striking demonstration of their possible supramolecular organization [2]. At the same time there are a number of works, which present the evidence of a rhodopsin monomeric state in the photoreceptor membranes [3,4].

We have investigated the rhodopsin supramolecular organization in the photoreceptor membranes in the solution by small angle X-ray (SAXS) and neutron (SANS) scattering methods. SANS experiments were performed with the various parts of heavy water in the solution (contrast variation method) to obtain the information about the lipid and the protein components separately. It was shown that the packing density of the rhodopsin molecules in the photoreceptor membrane is unusually high. The distance between the centers of the molecules is approximately 56 Å. The probability of the monomeric state of rhodopsin molecules in the photoreceptor membrane, according to our data, is rather high [5].

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V.N. Pribora

OOO Bruker, Moscow, Russia
vasily.pribora@bruker.com

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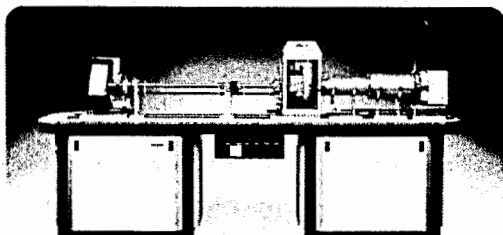


Fig.1. System for SAXS NANOSTAR

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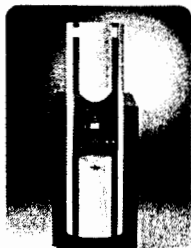


Fig.2. System for SAXS with vertical layout N8 HORIZON

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Our N8 HORIZON (Fig.2) is the ideal solution for the characterization of solid-state nanomaterials. It possesses a revolutionary vertical beam path with an impressively small footprint.

The compact MICROpix (Fig.3) and MICROcaliX series features the renowned Kratky-design, with a particular focus on highest measurement speed, precision and user convenience. The MICROcaliX uniquely combines microcalorimetry and SAXS in a single instrument and is designed in particular for the characterization of temperature sensitive materials, such as liquid crystals, fats, polymers, protein gels and pharmaceuticals.



Fig.3. Table-top SAXS and WAXS MICROpix

Bruker's in-house systems provide a level of data quality so far only achievable with much stronger synchrotron radiation source, making the in-house method a more attractive solution than ever.

Small-angle neutron scattering study of hydrocarbon-responsive surfactant micellar networks

A.V. Shibaev¹, A.V. Rogachev^{2,3}, A.I. Kuklin^{2,3}, O.E. Philippova¹, A.R. Khokhlov¹

¹ Moscow State University, 119991 Moscow, Russia

² Joint Institute for Nuclear Research, 141980 Dubna, Russia

³ Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Russia

shibaev@poly.phys.msu.ru

Surfactant molecules can self-assemble and form long cylindrical or wormlike micelles which behave like “living” polymers and form a transient network with viscoelastic properties. Due to their self-assembled nature surfactant micellar networks are highly responsive to external stimuli, e.g. the addition of hydrocarbons, which can be easily solubilized by the micellar hydrophobic cores and thus affect the structure of the micelles. This is a key property for the application of viscoelastic surfactant solutions as a main component of hydraulic fracturing fluids in oil recovery. In the present work we investigate the hydrocarbon-induced structural transitions in the networks based on wormlike surfactant micelles of an anionic surfactant.

In this work, the whole range of structural transitions taking place upon addition of hydrocarbon to wormlike micelles is investigated. At very small hydrocarbon concentrations, the solutions are highly viscoelastic due to the presence of long entangled wormlike micelles. As shown by small-angle neutron scattering (SANS) [1], the local cylindrical structure of the micelles is not perturbed by solubilization of small amounts of hydrocarbon, which have only minor effect on the micellar persistence length. At slightly higher hydrocarbon concentrations, a coexistence of cylinders and spheres is observed, which indicates to the progressive disruption of cylindrical micelles and the appearance of small spherical microemulsion droplets, accompanied by the loss of viscoelastic properties [2]. The volume fraction and radius of spheres grow with increasing hydrocarbon concentration. Finally, at high hydrocarbon concentrations, cylindrical micelles are fully disrupted and only microemulsion droplets are present in the solution.

It is shown that mixing wormlike micelles with an associating polyelectrolyte induces the disruption of “flower-like” micelles formed by the polyelectrolyte in the absence of surfactant, and results in the formation of a viscoelastic network formed by both micellar and polymer chains. Upon the addition of hydrocarbon, the viscoelastic properties of such a network are completely lost. As shown by SANS, this is due to the disruption of the micellar component of the network, which, as in the case of “pure” micelles, proceeds by the mixture of cylindrical micelles and spherical microemulsion droplets. However, at high hydrocarbon concentrations

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“hybrid” microemulsion droplets are formed, which consist of a hydrocarbon drop stabilized by a surfactant layer with associated polyelectrolyte chains.

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Structure of Nanoporous Carbons as revealed by Small-Angle X-Ray Scattering and TEM

A.A. Shiryaev¹, V.V. Volkov², P. Pré³, A.M. Voloshchuk¹

¹ Institute of physical chemistry and electrochemistry, Moscow, Russia. shiryaev@phych.e.ac.ru

² Institute of crystallography, Moscow, Russia

³ GEPEA-CNRS laboratory, Mines de Nantes, France

Nanoscale structure heavily influences adsorption and transport processes of carbon materials. Nanoporous carbons exhibit a very disordered nanostructure, with a carbon backbone formed by assemblages of defective graphene sheets with cross-links, the pore morphology is irregular, leading to more or less broad pore size distributions and possibly, partially closed porosity. Small-angle scattering (SAS) is often used in studies of porous materials, but complexity of their structure makes unique interpretation of obtained results difficult in many cases. In particular, evaluation of SAS studies of activated carbons is usually performed in assumption of atomically flat pore boundaries of graphene layers. This assumption is largely based on two famous papers devoted to investigation of fibers-based carbons using SAS and TEM [1, 2]. However, recent high resolution TEM studies of various carbonaceous sorbents [3] clearly show that generalization of this assumption to all carbonaceous materials is a gross oversimplification.

The aim of the current study was to explain the differences observed in the nanoporosity of a variety of activated carbons using the information collected about their structure. The set of adsorbents under investigation includes both commercial and non commercial activated carbons, produced from a variety of resources, as well as a carbon molecular sieve. The FAS series is representative of different degrees of activation of carbons made from a synthetic monomer (furfural). Pore size and volume distributions were determined by conventional methods, from measurements of N₂-77K and CO₂-273K adsorption isotherms. Structural information was obtained from the combination of two characterization methods: Small and Wide Angle X-ray Scattering (SWAXS) and Transmission Electron Microscopy (TEM).

Detailed modeling of SAS patterns from objects with variable surface roughness was performed. These objects approximate complex morphology of pores observed by TEM in our samples. Some of furfural-based samples discussed in the current work were analysed using TEM protocol from [3] and it is obvious that many pores can not be approximated by a void formed by atomically flat walls. For example, some of the walls are formed by stacks of ruptured graphene layers for which the formalism of "sharp" interface is not applicable. In general case of a pore

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with rough/corrugated surface the deviations from the Porod law became significant and, at least partly, invalidate extraction of closed porosity values. In most cases the pore-matrix interface in the studied samples is not atomically sharp, but is characterized by 1D or 2D fluctuations of electronic density responsible for the deviations from the Porod law. Depending on exact topology of the wall, its roughness may influence the scattering curve similar to mathematically-derived effects of finite thickness of the void-matrix interface or fluctuations of electron density (e.g., [4]).

It is shown that the intensity of the pores-related scattering correlates positively with S_{BET} values obtained from N_2 adsorption. Based on comparison of experimental and theoretical SAS patterns with structural data from TEM we discuss applicability of Porod law to interpretation of SAS studies of carbons and suggest consistent interpretation of the structural data and their relation with adsorption properties.

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How to get D₂O/H₂O contrast estimation from all-atom molecular dynamics trajectories for large biomacromolecular complexes

A.V. Shvetsov^{1,2}, M.A. Koltsov^{1,3}, D.V. Lebedev¹, V.V. Isaev-Ivanov¹

¹ Petersburg Nuclear Physics Institute, NRC "Kurchatov Institute", Gatchina, Russia

² Peter the Great Saint-Petersburg Polytechnic University, Saint-Petersburg, Russia

³ Saint-Petersburg University, Saint-Petersburg, Russia

alexxy@omrb.pnpi.spb.ru

SANS is a common technique that can be used to study different types of biological systems in solution. In case of large molecular complexes using only SANS methods can yield limited information about the structure of such systems. This limitation can be eased by using theoretical methods such as molecular dynamics simulations. While the advances in molecular dynamics methods and computer hardware allow for realistic simulation of dynamics of large macromolecules, it is always questionable whether the model of complex biomacromolecular system works as it can be found in experiment. Taking these two methods into account allows us to create and verify all-atom models even for large and complex molecular system.

A method to calculate SANS[1] and NSE[2] curves from MD trajectories was developed and implemented as analysis modules for molecular dynamics software package GROMACS. Previously other groups proposed methods to estimate contrast for small systems such as fatty-acids in organic non-polar solutions[3]. We extended method that was previously developed[1,2] to include D₂O/H₂O contrast estimation directly from molecular dynamics trajectories. This new technique was applied to systems containing DNA and protein parts (Fig. 1).

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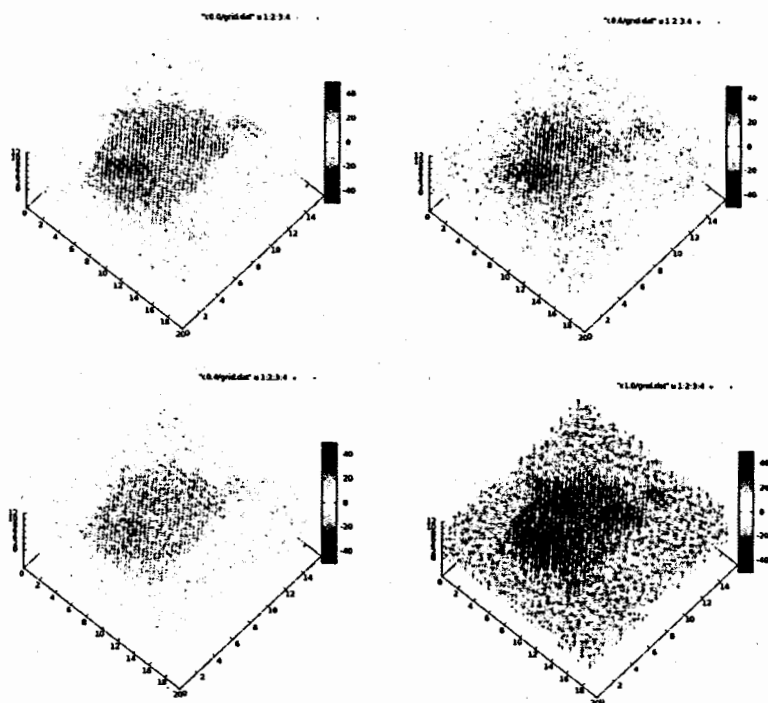


Fig. 1. Neutron scattering length density map for Nucleosom with DNA in water at different D₂O/H₂O levels (top left 0.0, top right 0.6, bottom left 0.4, bottom right 1.0).

Fractal aggregates of polydisperse particles with tunable dimension

O.V. Tomchuk^{1,2}, M.V. Avdeev¹, L.A. Bulavin²

¹ FLNP JINR, Dubna, Russia

² Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

tomchuk@jinr.ru

The wide range of nanomaterials is of great practical importance because of their unique physical-chemical properties due to the outstanding specific area values. Effective diagnostics of relevant industrial products as well as the prediction of their features require detailed knowledge of structure. Frequently nanoparticles are collected into fractal aggregates, which demands consideration of complex scale-invariant systems describing by statistical law, that can be presented, for example, as:

$$N = k(R_g/a)^D, \quad (1)$$

where a is the primary particle mean radius, N is the number of aggregate particles, k is so-called fractal prefactor, and R_g is the gyration radius of aggregate. Fractal (Hausdorff) dimension D is an essential feature of any self-similar fractal, characterizing as a measure of the space-filling capacity.

The scale-invariant structure of aggregates determines their dynamic properties such as translational friction, sedimentation and diffusion which are of interest in polymer science and biophysics. Size-dependent surface areas are of interest for colloidal chemistry. Scaling (1) has influence on scattering and absorption of various radiations, on transfer of heat and momentum between particles and carrier, on electron paramagnetic resonance and so on.

Prediction of the physical properties of aggregates is dependent on aggregate internal structure, so it should be based on precise experimental analysis of the statistically representative ensemble of aggregates. A much efficient way implies the numerical generation of fractal clusters using different deterministic and stochastic algorithms. Often nanoparticles are not monodisperse, and their sizes are distributed over some range. In this paper, a new model of fractal aggregates of polydisperse particles is given. The non-kinetic algorithm, able to construct the stochastic fractal clusters of polydisperse particles with tunable structural parameters, is presented. Model is based on a hierarchical procedure and allows covering the full range of fractal dimensions (1-3). The morphology study of the numerically generated aggregates is based on correlation analysis in direct space as well as in reciprocal space. It is shown that all previously

Contributed Talks

described analytical algorithms of fractal generation are limit cases of the presented general model. It is very useful for analysis of polydispersity-dependent as well as dimension-dependent structural features of fractal clusters. Also our goal is to give an analysis of scattering by such systems as an example of practical application of the developed algorithm.

Small angle and wide angle x-ray scattering study of boron clusters: interparticle correlations

A.N. Zhigunov¹, P. Matejcek²

¹ Institute of Macromolecular Chemistry, v.v.i., Academy of Sciences of the Czech Republic, Prague, Czech Republic

² Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czech Republic
zhigunov@imc.cas.cz

In this study, we have followed the behavior of anionic boron hydrides. Interparticle distances were measured for a wide range of concentrations by means of small angle x-ray scattering (SAXS) and wide angle x-ray scattering (WAXS). For our study, we have chosen boron clusters B12 ($[B_{12}H_{12}]^{2-}$) with Na cations and clusters CB11 ($[CB_{11}H_{12}]^{-}$) with K cations. Compounds based on boron clusters could be used for the treatment of a broad variety of biological targets including the inhibition of HIV protease, and others. Possible arrangements and aggregation behavior of these clusters are important for an understanding of its potential role in medical applications. Based on results obtained from concentration dependence we propose a model which comprises two levels of aggregation. In WAXS region correlation peak arises with concentration increase. This peak corresponds to the distance ~ 5 Å, which is slightly smaller than the diameter of single cluster, but larger than the distance between farthest B atoms. This is a question of mutual orientation of boron clusters and probably represents the lowest possible distance between boron clusters in small aggregates (SA). This is in agreement with the model proposed by Jae-Hyuk Her et al. based on crystallographic results [1]. In SAXS region we observe another level of association, which is seen as structure peak at $q = 0.36 \text{ Å}^{-1}$ for the concentration 0.6M. This peak is not observed for lower concentrations and for higher concentrations it shifts towards lower angles. Similar behavior was observed by W. Hausler et al [2] for Apoferritin in aqueous solution. This is a second level of aggregation as a result of SA association.

Acknowledgment: Support by the Czech Science Foundation (Project 14-14608S) is gratefully acknowledged.

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POSTER SESSION

Beta-lactoglobulin self-assembly: a small angle neutron scattering study

L. Anghel¹, R.V. Erhan^{2,3}

¹ Institute of Chemistry of Academy of Sciences of Moldova, Chisinau, Republic of Moldova

² Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Magurele, Romania

³ Joint Institute for Nuclear Research, Dubna, Russian Federation

anghel.lilia@gmail.com

The monomeric β -lactoglobulin (β -lg) is a small globular protein a molecular weight of 18.4 kDa, member of the lipocalin family of proteins [1]. This protein consists of a single polypeptide chain of 162 amino which are organized into 8-stranded antiparallel β -barrel with a 3-turn α -helix on the outer surface and a ninth β -strand flanking the first strand (Fig. 1).

β -lg was identified in the milk of many mammalian species, excepting the human, lagomorphs and rodent milks, where it was absent. It was established that β -lg is the main fraction of the whey protein in bovine milk [2]. Although, this protein has been extensively studied, its biological functions are still unknown.

In aqueous solutions, β -lg undergoes aggregation processes as a result of various conditions [3]. The study of homo-association (Fig. 1) and formation of oligomeric states of β -lg will give some insights into the functional properties of this protein. We have studied the influence of pH and concentration on aggregation process and the morphology of β -lg aggregates. In all cases, small angle neutron scattering was essential to determine the three-dimensional models of the homo-associates of β -lg.

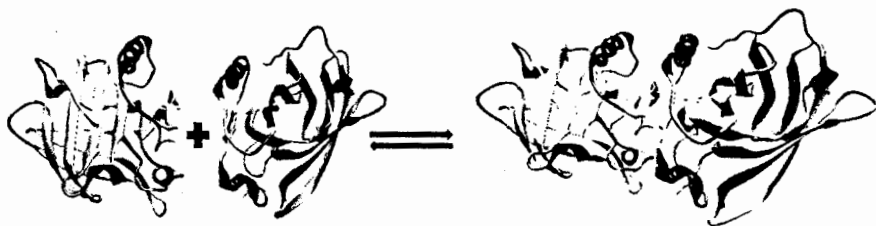


Fig. 1. Graphical representation of unliganded monomeric form of bovine β -lactoglobulin (PDB entry 5IO5) and its homo-dimer.

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Measurements on the collagen by neutron contrast variation

D. Aranghel^{1,2}, C.R. Badita^{1,3}

¹ National Institute for Nuclear Physics and Engineering, Reactorului 30, RO-077125, POB-MG6 Bucharest-Magurele, Romania

² Extreme Light Infrastructure Nuclear Physics (ELI-NP), Reactorului 30, RO-077125, POB-MG6, Bucharest-Magurele, Romania

³ University of Bucharest, Faculty of Physics, Atomistilor 405, CP MG - 11, RO - 077125, Bucharest-Magurele, Romania

daranghe@nipne.ro, ramona@tandem.nipne.ro

The principle of Small-Angle Neutron Scattering (SANS) contrast variation is applied to characterization of type I collagen protein from bovine achilles tendon. Contrast variation is used to determine the incoherent part of the scattered intensity which is subtracted subsequently from the measured intensities [1]. By varying the composition of the D₂O/H₂O solvent, a “contrast match” solvent composition is identified for which the scattered intensity is minimized. This solvent mixture is subsequently used to SANS experiments on collagen solutions for estimating the collagen matrix density and the pore size distribution [2]. It is well known that the apparent radius of gyration varies with the scattering density of the solvent [3].

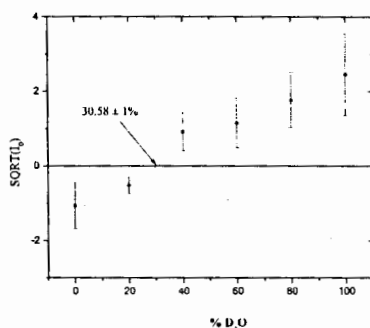


Fig. 1. Type I collagen from bovine achilles tendon concentration 15mg/ml

Different collagen concentrations in D₂O solvent were measured in order to understand the relationship between the conformation and structure parameters of collagen molecule in solution.

The contrast matching point of type I collagen from bovine achilles tendon, powder, Figure 1, was determined to be $30.58 \pm 1\%$, corresponding to a scattering length density $\rho_{\text{collagen}} = 0.913 \cdot 10^{-6} \text{ \AA}^{-2}$.

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SANS-study of carbon matrices made by pyrolysis of bis-phthalocyanines of metals used for storage and transmutation of radioactive waste

V.Y. Bairamukov¹, V.T. Lebedev¹, V.I. Tikhonov¹

¹ National Research Centre "Kurchatov Institute" B.P. Konstantinov Petersburg Nuclear Physics Institute,
Orlova Roscha, Gatchina, Leningrad district, 188300, Russia
vbayramukov@gmail.com

New type of carbon matrices for a long-time storage of nuclides has been created and studied by SANS to get the information on subtle details of metal atoms encapsulation. The problem of conditioning, storage and transmutation of radioactive waste (RW), containing long-lived isotopes, including minor actinides, calls for creation of new chemically and thermally stable matrices resistant to ionizing radiation. Carbon-based matrix appears to be most suitable in meeting such hard requirements. Carbon is chemically resistant, can withstand high thermal loads, and both of its stable isotopes (C^{12} and C^{13}) have low neutron capture cross-sections (3.4 and 1.3 mb) that is especially important for the process of transmutation. Particularly, the method of manufacturing matrices for storage and transmutation of RW containing minor actinides that is based on pyrolysis of their bis-phthalocyanines has shown very promising results during initial tests of the chemical, thermo and radiation stability.

The structure of carbon matrices prepared from bis-phthalocyanines by pyrolysis when the metal atoms were captured inside small cells as a result of thermal treatment at 800–1700°C [1] was studied. As it was shown, the structure of these substances at the scales $\sim 10^0$ – 10^2 can be characterized when we consider three structural levels, i.e. very small cells (~ 1 nm), their groups (~ 3 – 10 nm) and large aggregates (≥ 100 nm) composed of groups. The amount and size of these scattering elements has increased by annealing at the temperatures above 1000°C. The SANS data are in agreement with atomic force microscopy results [2].

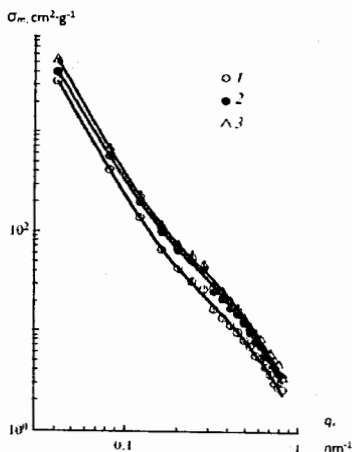


Fig. 1. SANS patterns for annealed sample YC_x: 1 – TA = 850°C, 2 – TA = 1350°C, 3 – TA = 1700°C; a – the dependence of neutron scattering cross section on momentum transfer q . Lines show the data approximation by model scattering functions

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Neutron depolarization method applied for magnetorheological elastomers investigations

M. Balasoiu^{1,2}, S.V. Kozhevnikov¹, Yu.V. Nikitenko¹, V. Birsan², I. Bica³, M. Bunoiu³

¹ Joint Institute for Nuclear Research, 141980, Dubna, Russia

² "Horia Hulubei" National Institute of Physics and Engineering, P.O. Box.MG-6, Bucharest, Romania

³ West University of Timisoara, Department of Physics, 300223, Timis, Romania

balas@jinr.ru

Magnetorheological (MR) elastomer [1, 2], known as "smart and intelligent materials", is generally achieved from an elastic matrix such as natural rubber and silicone rubber, in which magnetizable particles are dispersed and/or aligned. Rheological properties of the MR elastomer can be tuned by controlling the intensity of the applied magnetic field. Their mechanical properties, including the elastic characteristics and rheological properties, are sensibly influenced by the application of an external magnetic field. In contrast, in the case of MR fluids, the magnetizable microparticles are dispersed in liquid media such as silicone oil and mineral oil, similar to electrorheological fluids under an electric field applied. While in the MR elastomers, the magnetizable component lays inside the elastic matrix, such as silicone rubber, natural rubber, polyurethane sealant, acrylonitrile, and polybutadiene; unlike the MR fluids, magnetic particles in the MR elastomers do not settle inside the matrix. MR elastomers can be produced either in the absence or in the presence of the magnetic field. Without magnetic field, an isotropic MR elastomer is produced, while anisotropic MR elastomers are produced in the presence of the magnetic field. Mechanical characteristics of tension and deformation, viscoelastic properties, and magnetostrictive effect of the MR elastomers can be continuously and reversibly modified in a few milliseconds with and without an applied external magnetic field, making the MR elastomers susceptible for various applications including electric current passive and active elements, adaptive tuned vibration absorbers, resonator absorber, and seismic protection.

In the present paper we report the investigation of static magnetic fluctuations inside magnetorheological elastomer samples by means of neutron depolarization method [3,4].

Acknowledgments This work was supported by the JINR-Romania Scientific Projects Nos. 95/15.02.2016 items 47, 90, and 96/15.02.2016 items 47, 90 and the Grant of the Romanian Governmental Plenipotenciary at JINR No.94/15.02.2016 item14.

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Synchrotron powder diffraction investigations of biogenic ferrihydrite particles transformations induced by variation of the growth conditions for the microorganisms

S.E. Kichanov¹, M. Balasoiu^{1,2}

¹ Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, Russia

² Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania
balas@jinr.ru

Synchrotron radiation sources have several advantages over conventional X-radiation sources, including a wider spectrum and higher luminosity. This is the reason why synchrotron radiation has been increasingly used in the world to solve a wide spectrum of fundamental and applied problems in physics, chemistry, materials science, biology, medicine and earth sciences. At the experimental station "Mediana" of the Kurchatov Synchrotron Radiation Source, a diffractometer for investigations of microsamples with the help of synchrotron radiation has been created [1].

One of the topical problems to be solved with the help of synchrotron radiation is the investigation of the structure and phase diagrams of condensed matter. High intensity of the synchrotron radiation beam allows carrying out experiments with small volumes of the investigated matter.

Samples Fe12 (A) and Fe34 (B) separated from a bacterial biomass grown during 8 and 21 days, respectively have been measured [2].

The investigated samples were positioned in a monochromatic beam with a wavelength of 0.586 Å. The data collection of diffraction patterns was done by means of Image plate type detectors.

Synchrotron diffraction spectrum of biogenic ferrihydrite nanoparticles (A) obtained at "Mediana" station (KSRS) are presented in Fig.1. Processing results of presented diffraction spectrum part in Fig.1 using a model of the cubic cell is shown in Fig. 2.

Diffraction peaks from the sample are located at scattering angles of $2\theta = 5,4^\circ; 8,1^\circ, 16^\circ$. Besides this, around the scattering angles of $2\theta = 10^\circ-13^\circ$ is observed a diffusive halo.

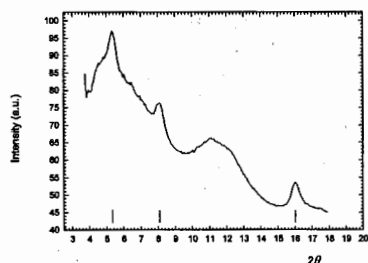


Fig.1. Diffraction spectrum of biogenic ferrihydrite nanoparticles obtained at "Mediana" station of the Kurchatov Synchrotron Radiation Source (KSRS).

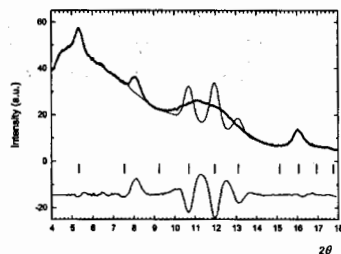


Fig.2. Processing result of obtained diffraction spectrum part (Fig.1) using the model of cubic cell.

The positions of the diffraction peaks which are related to each other as 2:3:6 may correspond to the cubic system. However, in this case, the description yields only the two extreme peaks of the spectrum. These positions are consistent with the values of Miller indices (100) and (300). The peak located at a scattering angle $2\theta = 8,1^\circ$ is located close to the position corresponding to Miller indices (110).

In the present paper the results on both samples A and B are presented and discussed.

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SANS investigation of magnetic polydimethylsiloxane elastomers polymerized in different oriented magnetic fields

M. Balasoiu^{1,2}, V.T. Lebedev³, I. Bica⁴, M. Bunoiu⁴, A.V. Rogachev^{1,5}

¹ Joint Institute for Nuclear Research, Dubna, Russian Federation

² Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest, Romania

³ Petersburg Nuclear Physics Institute, Gatchina, Russian Federation

⁴ West University of Timisoara, Department of Electricity and Magnetism, Timisoara, Romania

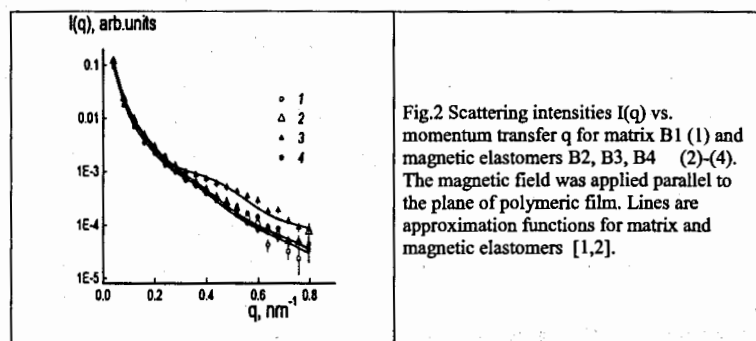
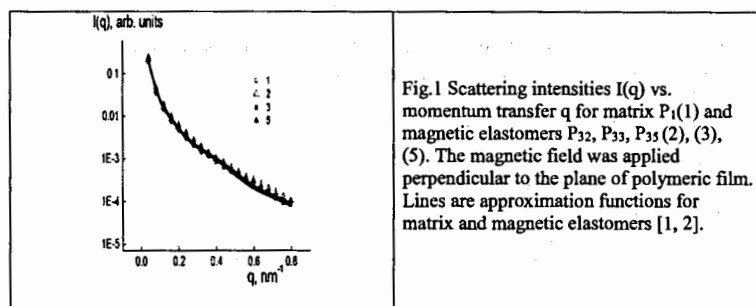
⁵ Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia

balas@jinr.ru

Magnetic elastomers were prepared using the radical polymerization of polydimethylsiloxane with addition of transformer oil based ferrofluid with magnetite particles. In the samples the concentration of magnetic component (ferrofluid) was: (i) 1.27 and respectively (ii) 1.64 wt %. The magnetic field was applied (i) perpendicular ($B = 0, 280, 560, 1120$ G) and was applied (ii) parallel to the plane of polymeric film ($B = 0, 377, 1131$ G). The samples thickness was of ~ 0.5 mm. It was prepared also the polymeric matrix without ferroparticles (reference sample).

The small angle neutron scattering experiments (SANS) have been carried out at ambient temperature (20°C) on the diffractometer "Membrane" (PNPI) in the range of momentum transfer $q = (4\pi/\lambda)\sin(\theta/2) = 0.03 - 0.8 \text{ nm}^{-1}$ where θ is scattering angle and $\lambda = 0.3 \text{ nm}$ is neutron wavelength ($\Delta\lambda/\lambda = 0.25$). In all the experiments there were studied the samples being isotropic in scattering plane. The incident beam was orthogonal to the planes of elastomers' films. Thus, the scattered intensities were dependent on the modulus q of scattering vector only. Since the neutron beam transmission for the samples was relatively high, $Tr \sim 0.8$, the multiple scattering processes can be neglected.

The scattering intensities and the model fittings are presented in Fig.1 and Fig.2.



The structural features of the magnetic elastomers polymerized in the magnetic field of perpendicular and parallel orientation to the plane of polymeric film are obtained.

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SANS investigations of Ti-Ag thermionic vacuum arc deposition

R. Vladoiu¹, M. Balasoiu^{2,3}, D. Soloviev^{2,4,5}, A. Mandes¹, V. Dinca¹

¹ Department of Plasma Physics, Faculty of Physics, Chemistry, Electronics and Oil Technology, Ovidius University, Mamaia 124, Constanta, 900527, Romania

² Joint Institute for Nuclear Research, Dubna, Russia

³ Horia Hulubei National Institute for Physics and Nuclear Engineering, Bucharest, Romania

⁴ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁵ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

balas@jinr.ru

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. Titanium based thin films are envisaged for surface coatings applications requiring low roughness, good smoothness and low friction coefficient.

In the present paper, for the first time a small-angle neutron scattering (SANS) investigation of the Ti-Ag material deposited on silicon substrate (Fig.1) by the TVA method is reported.

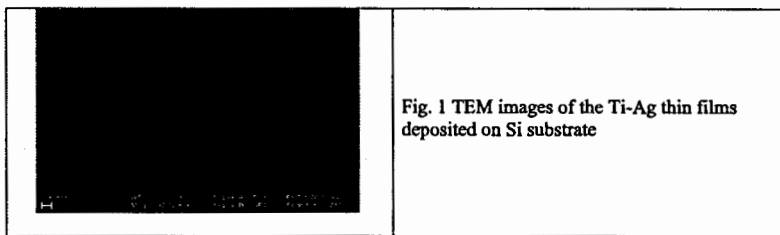


Fig. 1 TEM images of the Ti-Ag thin films deposited on Si substrate

In Fig.2 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) is presented.

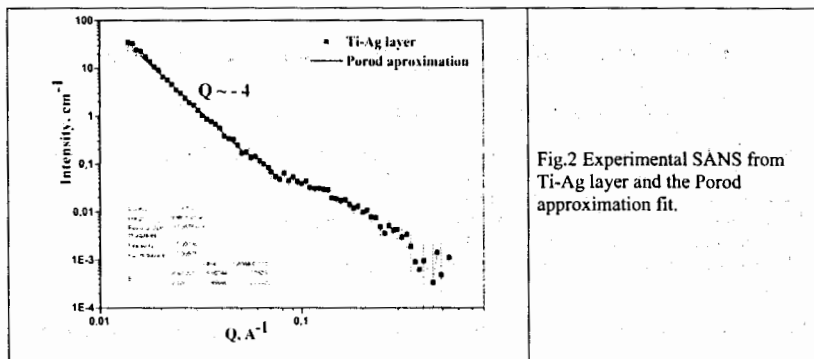


Fig.2 Experimental SANS from Ti-Ag layer and the Porod approximation fit.

The preliminary analyzes of the experimental data have shown that the characteristic SANS contribution from the Ti-Ag layer sample is in the range of $0.01 \text{ \AA}^{-1} \leq Q \leq 0.3 \text{ \AA}^{-1}$ (see Fig.1).

When two media are separated by a sharp interface, the scattered intensity follows an asymptotic law in the Q region: $I(Q) = AQ^{-\alpha} + B$. This law is called the Porod's limit.

The experimental curve obtained from the measured sample reveals in the Q range of $0.015 \div 0.07 \text{ \AA}^{-1}$ a such behavior with the Porod exponent $\alpha = 4$. This asymptotic value, when the contrast of the sample is known, and when the intensity is expressed in absolute scale, allows calculating the specific surface S of the particles.

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Concentration effects in cobalt ferrite/lauric acid-sodium dodecyl sulphate/water ferrofluid studied by means of SANS

M. Balasoiu^{1,2}, D.V. Soloviev^{1,3,4}, A.-M. Balasoiu-Gaina^{1,5}, O.I. Ivankov^{1,3,4}, N. Lupu⁶

¹ Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, Russia

² "Horia Hulubei" National Institute of Physics and Nuclear Engineering, Bucharest, Romania

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁴ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁵ West University of Timisoara, Department of Physics, Romania

⁶ National Institute of Research & Development for Technical Physics, Iasi, Romania

balas@jinr.ru, alexandra@balasoiu.com

Ferrofluids, known also as magnetic fluids, reveal a wide range of applications in many technical and industrial fields, as well as in medicine and biotechnology. 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 effects on the structure variation of a non-ionic CoFe_2O_4 /lauric acid/DDS-Na/ H_2O ferrofluid investigated by means of small angle neutron scattering are presented. Earlier results on the CoFe_2O_4 /lauric acid/DDS-Na/ H_2O ferrofluid sample of 3% particle volume concentration were reported. TEM images reveal that though the sizes and the geometrical forms are not uniform, the particles partially show rhomboidal shape. The model fit of SANS data gives triaxial ellipsoid and ellipsoidal shell, as objects characterizing the investigated system [3].

SANS data sets of 1%, 0.5% and 0.04% particle vol. concentration samples were obtained. The scattering curves were analyzed using model calculations included in ATSAS Package (GNOM, DAMMIN, DAMAVER) program [4]. It was accomplished the ab initio analysis aiming the recovering of three-dimensional structure from one-dimensional scattering curve for all the particle concentrations.

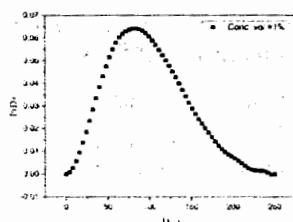


Fig.1 Size distribution function $P(D)$ for the ferrofluid sample of 1 % particle vol. concentration.

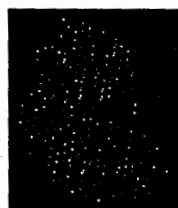


Fig.2 *Ab initio* reconstruction of overall CoFe_2O_4 nanoparticles shape for the ferrofluid sample of 1 % particle vol. concentration.

In Figs.1, 3 and 5 the size distribution for 1 %, 0.5 % and respectively 0.04 % particle vol. concentration samples are given, whereas in Figs. 2, 4 and 6 the corresponding *ab initio* constructions of overall nanoparticles shapes are represented.

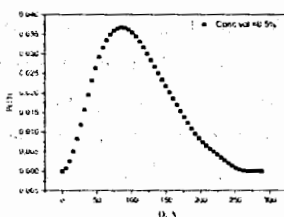


Fig.3 Size distribution function $P(D)$ for the ferrofluid sample of 0.5 % particle vol. concentration.



Fig.4 *Ab initio* reconstruction of overall CoFe_2O_4 nanoparticles shape for the ferrofluid sample of 0.5 % particle vol. concentration.

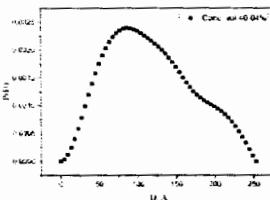


Fig.5 Size distribution function $P(D)$ for the ferrofluid sample of 0.04 % particle vol. concentration.



Fig.6 *Ab initio* reconstruction of overall CoFe_2O_4 nanoparticles shape for the ferrofluid sample of 0.04 % particle vol. concentration.

The variation of the size distribution and the mean size

Acknowledgements.

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Structural studies using small-angle neutron scattering of germante-lead glasses doped with silver oxide

V. Bodnarchuk¹, O. Pana², M. Rada², R.V. Erhan^{1,4}, R.-C. Suciu²,
N. Aldea², C. Leostean², S. Rada³, A. Kuklin¹

¹ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russian Federation

² National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania

³ Department of Physics & Chemistry, Technical University of Cluj-Napoca, 400020 Cluj-Napoca, Romania

⁴ Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Magurele, Romania

bodnarch@nf.jinr.ru

The $x\text{-Ag}_2\text{O} \cdot (100-x) [7\text{GeO}_2 \cdot 3\text{PbO}]$ glasses system up to 40 mol% of Ag_2O , were prepared and investigated by XRD and FTIR spectroscopies. The influence of Ag_2O content on optical properties and structure of the $7\text{GeO}_2 \cdot 3\text{PbO}$ glass network was investigated using fluorescence spectroscopy (PL) (Fig.1), X-ray diffraction (XRD) [1].

We report here small neutron scattering investigations using scattering neutrons (SANS) on these glasses and ceramic glass samples (Fig.2). The morphology of the film was studied by Scanning Electron Microscopy (SEM) and EDX measurements. The fluorescence spectroscopy data shows emission (red bands) lower than 2 eV are attributed to the presence of small silver nanoparticles [2].

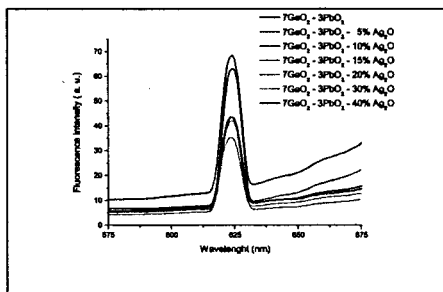


Fig. 1. Fluorescence measurements for $x\text{-Ag}_2\text{O} \cdot (100-x) [7\text{GeO}_2 \cdot 3\text{PbO}]$ with $x = 40$ mol%

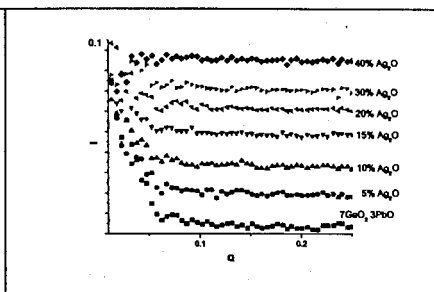


Fig. 2. Preliminary small-angle neutron scattering spectra of the studied systems.

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Study of carbon-supported bimetallic PtCu nanoparticles by ASAXS

N.V. Bulat, L.A. Avakyan, V.V. Pryadchenko, V.V. Srabionyan, S.V. Belenov., L.A. Bugaev

Southern Federal University, Rostov-on-Don
bulat@sfedu.ru

Catalysts, which are based on Pt nanoparticles, are widely used as in many practically important reactions, including reactions of hydrogen electro-oxidation in low-temperature fuel cells [1]. By forming bimetallic Pt-M nanoparticles with core-shell structure, it is possible to reduce the cost of electrocatalyst, as well as to improve its stability during the operation [2]. The experimental small-angle X-ray scattering data (SAXS) were collected at the synchrotron BESSY-II (Berlin, Germany). The spectra of small-angle scattering are a powerful instrument for studying the structure of materials at an intermediate scale range between the atomic structure of matter (1-10Å), studied by indirect methods and mesoscopic scales which are accessible for direct observation techniques [3]. The information about the structure of the nanoparticles at atomic and over atomic levels is important for establishing the relationship between synthesis parameters and catalytic properties of the material. Particularly the interest is in the size distribution of nanoparticles, the structure of their inner regions, composition, thickness, and continuity of the near-surface region. Study of the size distributions can be carried out by fitting or by molecular modeling using the Monte Carlo method. The information about the structure of PtCu nanoparticles was derived from experimental data and the average thickness of Pt shells was evaluated. The study was performed with the support of Grant № 213.01.-07.2014/10ПЧБГ of Southern federal university.

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Ultrastructure of heart mitochondria studied by SANS and SAXS

I.M. Byvshev¹, I.M. Vangeli², T.N. Murugova^{1,3}, O.I. Ivankov^{1,3,4},
A.I. Kuklin^{1,3}, V.I. Popov⁵, V.V. Teplova⁵, L.S. Yaguzhinsky^{1,2}

¹ Moscow Institute of Physics and Technology, State University, Dolgoprudnyi (Russian Federation)

² A.N. Belozersky Institute of Physico-Chemical Biology, Moscow (Russian Federation)

³ Joint Institute for Nuclear Research, Dubna (Russian Federation)

⁴ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁵ Institute of Cell Biophysics, Russian Academy of Sciences, Pushchino (Russian Federation)

ivan.byvshev@gmail.com

It is well known that complexes of oxidative phosphorylation (OXPHOS) system could operate structurally in two states – in state of supercomplex and in dissociated state. Earlier on liver mitochondria it was found that supercomplex regime is realized under conditions of normal and low tonicity, while in high tonicity OXPHOS operates in dissociated state.

In present work using double-inhibition technique we have founded that in heart mitochondria OXPHOS system operates as a supercomplex at wide range of tonicities of incubation media (Fig. 1).

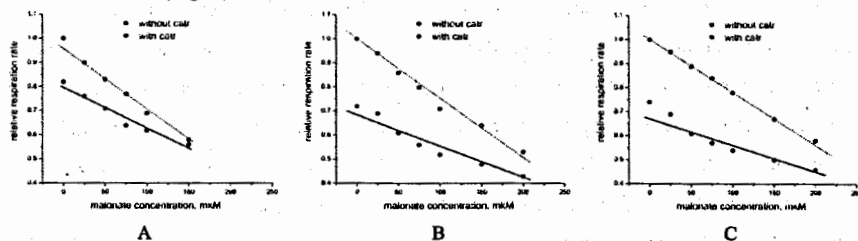


Fig. 1. Double-titration of respiration by malonate in absence and presence of CATR on heart mitochondria under hypertonic (600mOsm) – A, isotonic (300mOsm) – B, and hypotonic (120mOsm) – C, conditions.

The investigation of mitochondrial ultrastructure by method of small-angle neutron scattering (SANS) under conditions of normal tonicity (300mOsm – isotonic medium) and low-amplitude swelling (120mOsm – hypotonic medium) proved the existence of ordered membrane structures in mitochondria. The experiments were performed on YuMO spectrometer (IBR-2M, Dubna, Russia).

SANS measurements were carried out on dense mitochondrial suspension. It was shown that under both isotonic and hypotonic conditions the highly-organized structures are formed mitochondrial membrane. The formation of such structures was studied by contrast variation method (the solvent contained 12, 42, 100 % D₂O). the most of scattering curves have structural

peaks. The values of structural parameters corresponded to these peaks are presented in the Table 1.

The comparison of data, obtained from the investigation of function and structure of mitochondria let us suggest the existence of two types of supercomplexes with different structural parameters.

Table 1. Structural parameters obtained by SANS method for mitochondria in different incubation media, Å.

D ₂ O part in a medium	100%	42%	12%
Hypotonic media	380	265	Not found
Isotonic media	250	230	100

We performed SAXS experiments on similar mitochondria samples as well. It was shown that SAXS curves exhibit the same behavior as SANS curves for the mitochondria in media based on 12%-D₂O (see the example in Fig. 2). In this case the protein component of mitochondria gives the main contribution to the scattering intensity.

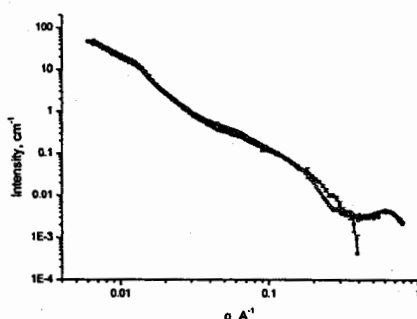


Fig. 2. SANS (○) and SAXS (■) scattering curves for rat heart mitochondria. SANS curve corresponds to mitochondria in 12%-D₂O medium.

SANS investigations of special aluminous cement matrices for conditioning of radioactive waste

A.C. Dragolici¹, M. Balasoiu^{1,2}, F. Dragolici¹, L. Ionascu¹, M. Micu¹, O.I. Ivankov^{2,3,4}

¹ Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania

² Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, Russia

³ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁴ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

balas@jinr.ru

The management of the radioactive waste implies the conditioning in a cement matrix as an embedding, stable, disposal material. Cement matrix is the first and most important engineering barrier against the migration in the environment of the radionuclides contained in the packages. Chemically, after mixing with water, cement produces a reacting matrix with a porous microstructure. Knowing how the microstructure develops is therefore desirable in order to assess the compatibility of radioactive streams with cement and predict waste form performance during storage and disposal. Adjustment of the phase fractions of the individual cement compounds in the anhydrous cement is one of the few means of altering its structural and mechanical properties.

The general aim of this research is to develop a modified cement system (Fig.1 and Fig.2) based on CEM III-A and CEM V-A by addition of aluminum sulfate to obtain the decreasing of portlandite concentration in shorter time by a direct chemical reaction during the setting time [1, 2, 3].

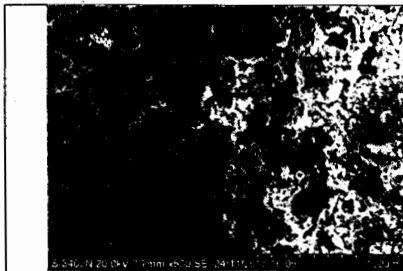


Fig.1 Scanning electron microscopy images of CEM III + H₂O cement sample.

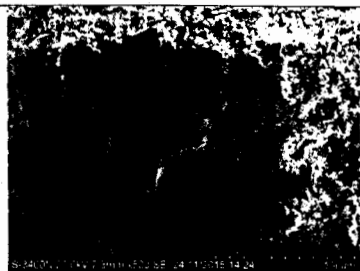


Fig.2 Scanning electron microscopy images of CEM III + H₂O cement sample.

Over the past 40 years, various small-angle x-ray scattering (SAXS) and small-angle neutron scattering (SANS) studies have been carried out to characterize and quantify the microstructures of complex cementitious materials [4-7].

In the present paper we present our preliminary SANS results on the samples:

I)

- 1) CEM V + H₂O
- 2) CEM V + H₂O + Al(powder)
- 3) CEM V + H₂O + Al(powder) + Al₂(SO₄)₃ + citric acid + pantarhol
- 4) CEM V + H₂O + Al(powder) + Al₂(SO₄)₃ + citric acid + pantarhol + LiNO₃

II)

- 1) CEM III + H₂O
- 2) CEM III + H₂O + Al(powder)
- 3) CEM III + H₂O + Al(powder) + Al₂(SO₄)₃ + citric acid + pantarhol
- 4) CEM III + H₂O + Al(powder) + Al₂(SO₄)₃ + citric acid + pantarhol + LiNO₃

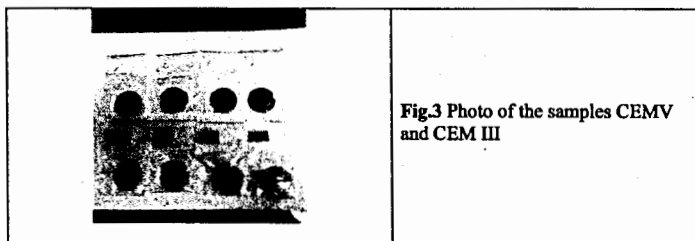


Fig.3 Photo of the samples CEMV and CEM III

Acknowledgments This work was supported by the JINR-Romania Scientific Projects Nos. 95/15.02.2016 item 122, and 96/15.02.2016 item 122 and the Grant of the Romanian Governmental Plenipotenciary at JINR No.94/15.02.2016 item10.

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Hetero-association of beta-lactoglobulin and sodium alginate studied by small-angle neutron scattering

L. Anghel¹, R.V. Erhan^{2,3}

¹ Institute of Chemistry of Academy of Sciences of Moldova, Chisinau, Republic of Moldova

² Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Magurele, Romania

³ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russian Federation
raul.erhan@gmail.com

B-lactoglobulin (β -lg) is the major whey protein abundant in cow's milk. *B*-lg is a lipocalin whose structure contains β -barrel with eight antiparallel β -strands and one major α -helix at the end of the molecule (Fig. 1). This protein has been widely used in the food and pharmaceutical industries due to its rheological and structural characteristics (e.g. unfolding, aggregation and gelation properties) [1].

B-lg is capable of binding various hydrophobic ligands, such as fatty acids and vitamins, carbohydrates, proteins and even inorganic elements [2]. At the present there is a gap with regard to the knowledge of β -lg and polysaccharides interactions. Such an understanding of the impact of interactions between β -lg and sodium alginate (Na-Alg) in food products and their biological functions will help to design food products with optimized nutritional properties. We have studied the influence of pH and molar ratio on the interactions between β -lg and Na-Alg mixtures. To solve the complexity of such systems and to determine the three-dimensional models of the obtained hetero-complexes, we have applied the small angle neutron scattering technique.

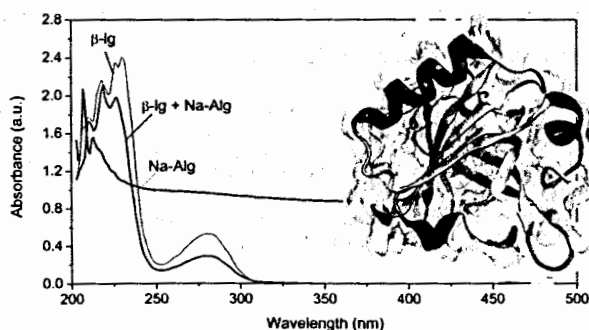


Fig. 1. UV-vis spectra of β -lg, Na-Alg and the mixture of β -lg and Na-Alg (1:1 ratio).

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Small-angle neutron scattering structural investigation of porous ceramic glasses

R.V. Erhan^{1,2}, M. Rada³, R.-C. Suci³, M. Zagrai⁴, S. Rada⁴,
E. Culea⁴, C. Leostean³, N. Aldea³

¹ Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, Magurele, Romania

² Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russian Federation

³ National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania

⁴ Technical University of Cluj-Napoca, 400020 Cluj-Napoca, Romania

raul.erhan@gmail.com

Small-angle neutron scattering (SANS) investigations on porous ceramics glass samples were carried out at YuMO SANS spectrometer, IBR-2 pulsed reactor.

It is known that germanate fibre optic materials are useful because they can work at long wavelengths (greater than 3 μm) and simultaneously with very low losses. Continuous Raman (study in progress), IR (Fig.1), UV-VIS and neutron scattering studies (Fig. 2) of lead containing germanate systems will lead to a full understanding of the fine features of the short- and medium-range order.

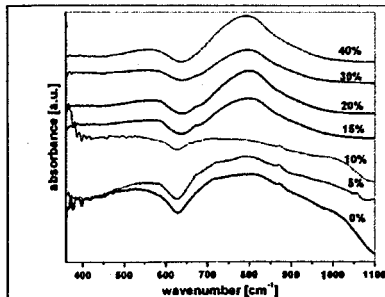


Fig. 1. FTIR spectra of the $x\text{Li}_2\text{O} \cdot (100-x) \cdot [7\text{GeO}_2 \cdot 3\text{PbO}]$ system where $0 \leq x \leq 40$ mol% Li_2O [1].

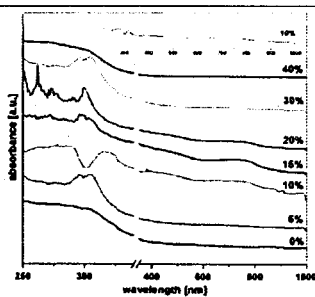


Fig. 2. UV-VIS absorption spectra of the $x\text{Li}_2\text{O} \cdot (100-x) \cdot [7\text{GeO}_2 \cdot 3\text{PbO}]$ system where $0 \leq x \leq 40$ mol% Li_2O .

The analyses of the IR spectra with smaller lithium ions content ($0 \leq x \leq 10$ mol%) reveal that the accommodation of the network with the excess of oxygen ions is possible by the increase of the degree of polymerization of the lead-germanate network.

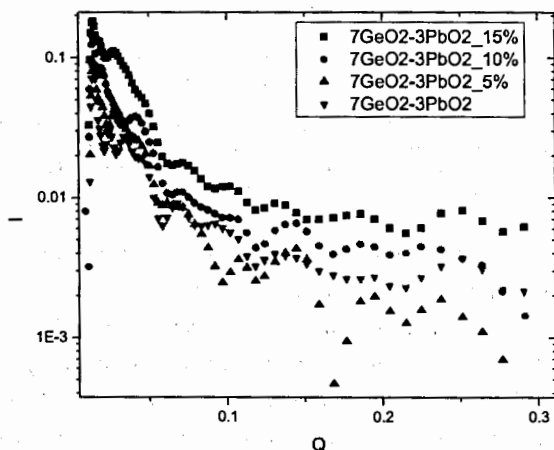


Fig. 3. Small-angle neutron scattering spectra of the studied systems.

We are looking to describe the nano-structure of the samples by obtaining the SANS standard parameters: the radius of gyration and a Porod exponents. A new Guinier– Porod analytical model will be introduced to fit SANS data of nano-particles embedded in amorphous glasses from spherical as well as non-spherical shapes such as rods or platelets.

Analysis of M-state of Bacteriorhodopsin D96N

A. Gapchenko¹, A. Vlasov¹, Yu. Ryzhikau¹, E. Zynoviev¹, Yu. Kovalev¹,
V. Borshchevskiy¹, V. Gordeliy¹, A. Kuklin^{1,2}

¹ Interdisciplinary Center for Fundamental Research, Laboratory for Advanced Studies of Membranes Proteins, Moscow Institute of Physics and Technology, Dolgoprudny, Russian Federation.

² Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russian Federation.
gapchenko@phystech.edu

In this work we show the results of SAXS measurements of gyration radius changes of D96N bR-containing purple membranes during light-induced M-state compared with its ground state. SAXS was done on the spectrometer Rigaku, MIPT, Dolgoprudny, Russia.

It was found that the strongest changes could be seen at alkaline pH values, higher than 8.5 [1,2]. In all our measurements we keep pH at 9.0 value. The concentration of purple membranes in samples was varied between ~20 mg/ml and ~2.5 mg/ml.

For high concentrations (10-20 mg/ml) the gyration radius changes wasn't noticed, possibly, due to the strong light absorption on the surface of capillary when in the middle of it there is no absorption and bR remains in the ground state, consequently there is fewer percentage of M-state induced BR molecules in relation to all amount of them.

For lower concentrations (5-2.5 mg/ml) the gyration radius changes were seen between 1.5-2.0Å. This indirectly approves the hypothesis of surface light absorption of bR in the capillary, but the reasons of the effect are being discussed.

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Structure stability of magnetic fluids in bulk and interfaces: combined analysis of small-angle neutron scattering and neutron reflectometry

I.V. Gapon^{1,2}, V.I. Petrenko^{1,2}, L.A. Bulavin², A.A. Vorobiev³, O. Soltwedel⁴, M. Balasoiu^{1,5}, L. Vekas⁶, V. Zavisova⁷, P. Kopcansky⁷, M.V. Avdeev¹

¹ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

² Kyiv Taras Shevchenko National University, Kyiv, Ukraine

³ Department of Physics and Astronomy, Uppsala University, Sweden

⁴ Max-Planck-Institut für Solid State Research, Stuttgart, Germany

⁵ National Institute of Physics and Nuclear Engineering, Bucharest, Romania

⁶ Center for Fundamental and Advanced Technical Research, Timisoara Branch RAS, Timisoara, Romania

⁷ Institute of Experimental Physics, SAS, Kosice, Slovakia

gapon@jinr.ru

Magnetic fluids (MFs) – fine stable dispersions of magnetic nanoparticles in liquids belong to the class of advanced nanomaterials. To ensure the long-term stability of MFs the magnetic nanoparticles are coated with some chemical layers, which prevent the particle coagulation because of the attractive van der Waals and magnetic interactions. Since 1960s MFs have been widely used in various industrial and technical fields. The present-day interest to these systems is also associated with their prospects in actively developing medical applications [1] such as drug targeting, magnetic resonance imaging (contrast medium), magnetic hyperthermia for cancer treatment, etc. For this purpose many efforts are concentrated on the synthesis of highly stable, reproducible and controllable water-based ferrofluids. In biocompatible colloidal systems for medical applications the chemical composition of the particle surface is of particular importance to avoid the action of the reticuloendothelial system, which is a part of the immune system, in order to increase the lifetime of magnetic nanoparticles in the bloodstream. If magnetic particles in MFs are coated with neutral and hydrophilic compounds such as poly(ethylene glycol) (PEG) [2], the latter increases from minutes to hours or days. There is a wide use of PEG in a great number of applications including the coating of colloidal particles of various origins [3] including those adsorbed at interfaces [4].

At the same time, the introduction of PEG into initially stable MFs can result in their structural reorganization. Such effect was recently observed [5] by small-angle neutron scattering (SANS) in bulk MFs where nanoparticles of magnetite (size below 10 nm) are placed in water and coated by double layer of sodium oleate (SO). In particular, comparatively small and compact nanoparticle aggregates (size at level of 40 nm) in the initial samples transfer to large (size above 120 nm) and developed (fractal dimension 2.5) associates after PEG (average molecular mass $M_w = 1000$ g/mol) is added to the system with the ratio above 2:1 with respect to magnetite

content [5,6]. It should be noted that smaller amount of added PEG did not lead to aggregates reorganization. The adsorption of PEG (hence, a partial substitution of SO) on the magnetite surface was proved by the infrared spectroscopy (IR) and differential scanning calorimetry (DSC). It is interesting that in accordance with the data of the SANS contrast variation it leads to minimal changes in the thickness of the stabilizing layer around magnetite nanoparticles as compared to the initial samples with SO only, thus reflecting the plane configuration of PEG at the magnetite surface. In the neat aqueous solutions PEG shows well the features of Gaussian coils [7]. The radius of gyration of the PEG coil is about 8 nm and the length of SO molecules is about 2 nm.

Neutron reflectometry experiments were done to investigate behavior of magnetic fluids with different methods of preparation and concentration at the interface with silicon. It was shown that individual nanoparticles are preferably adsorbed on the silicon surface. In MFs the interface shows the formation of just one well-defined adsorption layer of colloidal polydisperse particles from MFs. Adsorption layer was not observed after addition PEG to MFs, which was corresponded with decrease of the concentration of the single nanoparticles.

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Spectroscopic studies on biogenic ferrihydrite nanoparticles produced by bacteria *Klebsiella oxytoca*

C. Chilom¹, D. Gazdaru¹, G. Socol², A. Popescu¹, M. Balasoiu^{3,4}

¹University of Bucharest, Faculty of Physics, Romania

²National Institute for Laser, Plasma & Radiation Physics, Bucharest-Magurele, Romania

³Frank Laboratory of Neutron Physics, Joint Institute of Nuclear Research, Dubna, Russia

⁴Horia Hulubei National Institute of Physics and Nuclear Engineering, Bucharest, Romania

doina.gazdaru@gmail.com

Some spectroscopic properties of biogenic ferrihydrite nanoparticles produced by bacteria *Klebsiella oxytoca* were investigated. Dispersions in water and HEPES buffer of biogenic nanoparticles at different dilution were analysed by UV-Vis spectroscopy. Absorption spectra of diluted samples of the ferrihydrite nanoparticles show a large absorption in the 250 - 400 nm spectral range. The chemical composition of biogenic ferrihydrite nanoparticles was evaluated using FT-IR spectroscopy. Their FT-IR spectra revealed the typical absorption peaks characteristic to the exopolysaccharides. The exopolysaccharides can be present either on the surface and/or inside the pores of the ferrihydrite nanoparticles. Analysis on the basis of FT-IR spectroscopy shows also the characteristic peaks of amide groups present in proteins. However, the emission fluorescence spectroscopy does not confirm the presence of protein containing fluorescent amino acids in the sample. It is possible that some proteins to be present in the samples, but surely they do not contain fluorescent amino acids or they are in a very small quantity.

The intersect distribution of the tetrahedron: Approaches for simplification of cyclometric terms

W. Gille¹, S. Ciccariello²

¹ Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany

² Dipartimento di Fisica 'G. Galilei' e unita INFN, Padova, Italy
gille@physik.uni-halle.de

The intersect distribution of a homogeneous particle (sometimes denoted by chord length distribution, CLD) is a basic structure function in SANS [1]. For a convex particle, it is proportional to the second derivative of the correlation function. In recent years, starting from 2000, much work has been devoted to the tetrahedron case. It was shown by S. Ciccariello that the CLD, the probability density CLDD and the correlation function of a regular tetrahedron can algebraically be expressed in terms of elementary functions. Compared with the result for the cube, these expressions were relatively elaborate and long. Especially the result in [2] (2005) involves very many terms with inverse trigonometric functions.

Simultaneously, the tetrahedron has been investigated by W. Gille. As early as in 2003, this author published a simple approximation, see [3] and [1] p. 80. Here, the correlation function is given by polynomials - simplifying the full range of chord length intervals to two intervals. Contrary, the final result by S. Ciccariello involves an interval split into seven intervals, see [1] pp.78-80.

Until 2005, both authors worked independently on this matter. Furthermore, the long formula given in [1] was written down involving many substitutions and abbreviations.

During last years, the authors succeeded in simplifying these long expressions. In fact, now a very compact representation of the CLDD is available for application in SANS. Only seven cyclometric terms are involved. These terms directly reflect the five chord length intervals. This number of intervals is indispensable. Contrary to this, more complicated analytic representations required more intervals and even abbreviations for parametric integrals. The current calculations are based on the *Mathematica* system. New patterns for cyclometric functions were introduced.

The calculations were performed for the edge length $a=1$ of the tetrahedron. This is no restriction. The formulas can be transformed to any size of the body, see [1] p. 69. In contrast to the cube, the CLDD of the tetrahedron is a strictly monotonically decreasing function. This results from the four tips and six edges. Parallel interfaces do not exist. A Porod plot of the scattering intensity $I(q)$ does not involve oscillations.

Poster Session

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The role of small angle neutron scattering technique in transdermal drug delivery

T.L. Hangan¹, D. Badiu², S. Vladareanu³, D. Navolan⁴

¹ Department of Dermatology, Faculty of Medicine, "Ovidius" University of Constanta, Romania

² Faculty of Medicine, Ovidius University of Constanta, Romania

³ Elias University Hospital, 'Carol Davila' University of Medicine and Pharmacy, Bucharest, Romania

⁴ Department of Obstetrics-Gynecology and Neonatology, "Victor Babes" University of Medicine and Pharmacy Timisoara, City Emergency Clinical Hospital Timisoara, Romania

tonyhangan@yahoo.com, tony@medcon.ro

From ancient times the skin represents the membrane of drug application especially when different diseases are encountered. Therefore, the stratum corneum (SC) possesses a remarkable barrier to drug penetration. The SC is organized in lipid membranes arranged into a lamellar structure. Due to the special physicochemical properties of ceramides content, these membranes are very poorly permeable. In this respect, a number of skin diseases like atopic dermatitis, psoriasis or ichthyosis are related to an impaired structure of SC lipid membrane which could lead to an improper transdermal drug delivery. Recently, small angle neutron scattering (SANS) techniques have been applied describing the organization of SC structure. The present review highlights the role of SANS in transdermal drug delivery, concerning the investigations of the SC lipid membrane structure.

Keywords: neutron scattering, stratum corneum, transdermal, structure.

Neutron diffraction study of the crystal and magnetic structures of $\text{TlFe}_{1-x}\text{Ga}_x\text{S}_2$ compounds

R.F. Hashimov^{1,2}, E.B. Askarov^{1,3}, A.I. Beskrovniy¹, D.N. Toan^{1,4},
S.H. Jabarov², D. Neov¹, E.M. Karimova²

¹ Joint Institute for Nuclear Research, 141980 Dubna, Russia

² Institute of Physics Azerbaijan National Academy of Sciences, AZ-1143 Baku, Azerbaijan

³ National Nuclear Research Center, AZ-1143 Baku, Azerbaijan

⁴ Institute of Research and Development, Duy Tan University, 550000 Da Nang, Viet Nam
royshanhshimov404@gmail.com

Semiconductors with layered and chain crystal structures are a topic of current attention within the field of the solid state physics due to strong anisotropy of physical properties along the different crystallographic directions. The TlFeS_2 - TlGaS_2 system is one of such interesting compounds [1]. It was found that many members of this type exhibited the complex sequence of phase transformations, caused by a coexistence of long-periodic commensurate and incommensurate superstructures with changing temperature.

In order to study the effect of Ga^{3+} -doping at Fe^{3+} position on physical properties of TlFeS_2 we synthesized the following compositions of $\text{TlFe}_{1-x}\text{Ga}_x\text{S}_2$ ($x=0; 0.01; 0.025; 0.05; 0.075$). The crystal structure of the obtained samples was investigated by mean of X-ray diffraction method [3]. The X-ray diffraction result showed that the $\text{TlFe}_{1-x}\text{Ga}_x\text{S}_2$ system crystallized into a single-phase solid solution and the volume of unit cell decreased upon increasing the Ga-doping concentration. The increase of the gallium-doping content leads to a decrease of magnetization and an increase of magnetic phase-transition temperature [4].

This paper represents our results of the neutron diffraction studies of $\text{TlFe}_{1-x}\text{Ga}_x\text{S}_2$ in a large range of temperature. The neutron data diffraction analysis shows that all combinations of composition have the monoclinic crystal structure of $C2/m$ symmetry in all investigated temperature range. The formation of the long-range antiferromagnetic order of Fe ions was observed at low temperature. It was established that the Ga doping leads to the decrease of Neel temperature and magnetic moment of Fe ions. The temperature dependencies of structural and magnetic parameters were defined. Based on the obtained information the microscopic structural mechanism of magnetic ordering of $\text{TlFe}_{1-x}\text{Ga}_x\text{S}_2$ was established.

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Multifunctional Composite Materials

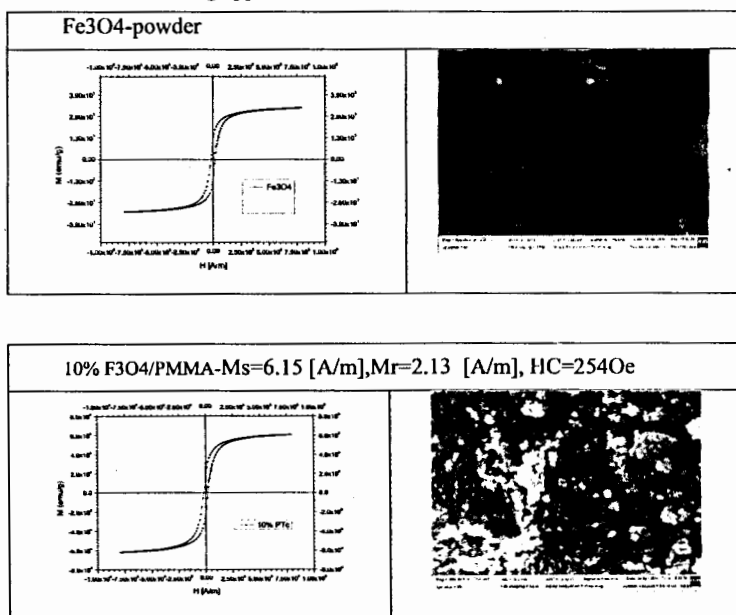
I. Ion¹, M. Lungu¹, V. Marinescu¹, D. Patroi¹, M. Lucaci¹, V. Thakiris¹, E. Mantea¹, M. Balasoiu², Yu.S. Kovalev², A.I. Kuklin², Yu. Nikitenko²

¹ INCDIEPE-CA, Bucharest, Romania

² JINR, Dubna, Russia

ion.ioana@icpe-ca.ro, carbonmat2016@gmail.com

In this work novel multifunctional materials with hierarchical structure are studied. Three concentration of magnetite respectively: 10, 40, 50 % in the PMMA matrix was synthesized in order to be used in the electromagnetic interference application. The composite materials present two hierarchical levels: micrometric beads consist on aggregated clusters of composite materials and magnetite nanoparticles with diameters ranging between 15-50 nm. The magnetic properties and structural characteristics were studied in order to obtain a better multifunctional composite material used in EMI shielding applications.



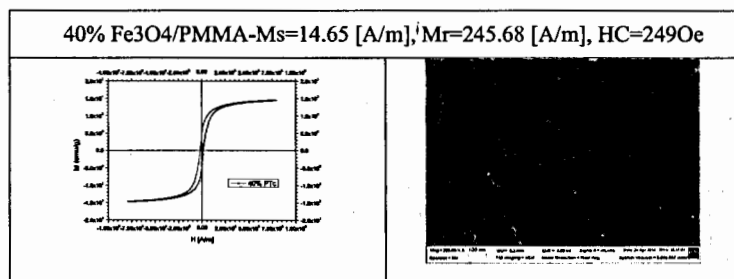


Fig. 1. Hysteresis and SEM micrographs of studied composite materials.

Silver behenate and silver stearate for better Q-scale SAS calibration

A.S. Kazantsev¹, A.V. Vlasov¹, Yu.L. Ryzhykau¹, O.I. Ivankov^{1,2,3}, D.V. Soloviov^{1,2,3},
E.V. Zinovev¹, A.V. Rogachev^{1,2}, Yu.S. Kovalev^{1,2}, V.I. Gordeliy^{1,2,4,5}, A.I. Kuklin^{1,2}

¹Laboratory for advanced studies of membrane proteins, Moscow Institute of Physics and Technology, Dolgoprudny, Russia

²Joint Institute for Nuclear Research, Dubna, Russia

³Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁴Institute of Complex Systems (ICS-6), Juelich, Germany

⁵Institut de Biologie Structurale J.-P. Ebel, Grenoble, France

alexander.iv.kuklin@gmail.com

vavplanet@mail.ru

It is well known that silver behenate (Ag-Bh) is widely used for SAS measurements calibration [1, 2]. In this work we suggest using the silver behenate (Ag-Bh) and silver stearate (Ag-St) mixed powder for providing better calibration when doing SAS experiments. The necessity of using the mixture of powders arises due to limitations of Q-scale dynamic range and two-parametric conditioning when not only the distance to detector is taken into account but also a wavelength in case of time-of-flight technique. In order to avoid the problem mentioned above as well as nonlinear scale effect of detectors we suggest using a mixture of silver behenate and silver stearate powders.

The feature of our method is that in case of using Ag-Bh/Ag-St powder mixture we can resolve twice more diffraction peaks than when using only Ag-Bh powder in the same Q-range due to closely located peaks. We calculated accuracy of this procedure.

In this work SAXS and SANS measurement results of silver behenate and silver stearate powders are presented and compared for two SAS-spectrometers: Rigaku, MIPT, Dolgoprudny (SAXS) [3] and YuMO, IBR-2, Dubna (SANS) [4, 5].

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Optical active nanoparticles in a silicate glasses: SANS studies.

S.E. Kichanov¹, V.S. Gurin², D.P. Kozlenko¹, O.I. Ivankov^{1,3,4},
A.Kh. Islamov¹, G.E. Rachkovskaya⁵, B.N. Savenko¹

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Research Institute for Physical Chemical Problems of the BSU, Minsk, Belarus

³ Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁴ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁵ Belarusian State Technological University, Minsk, Belarus

ekich@nf.jinr.ru

At present, the urgent problem of structural chemistry and materials science is to searching for optical materials with the possibility of varying their optical properties at the stage of synthesis.

One of 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. In our work most attention is focused on the research of structure aspects of optical properties formation in silicate glasses with different initial oxides $\text{TiO}_2/\text{CeO}_2$ molar concentration by means of small angle neutron scattering. The formation of complex oxide Ti-Ce-O nanoparticles in the silicate glasses was revealed. It is found that bounded regions of density fluctuation in the glass material without the addition of titanium and cerium oxides. These regions could serve as nucleation centers for oxide clusters of cerium and titanium upon their introduction into the matrix. Experimental results were explained by a model with two different types of nanoparticles formed in the silicate glasses. So at small molar concentrations ratio of initial $\text{CeO}_2/\text{TiO}_2$ oxides the nanoparticles are formed by predominately from oxygen, trivalent cerium Ce^{3+} and tetravalent titanium ions Ti^{4+} . With relative concentration $\text{CeO}_2/\text{TiO}_2$ 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.

Another small angle neutron scattering studies are investigations of glasses with semiconductor nanoparticles, which are convenient model objects for studying the effects of the interaction between light and quantum dots in the case where the sizes of the corresponding particles are in the range of the quantum limit. The study of optical materials based on glasses with nanoscale semiconductor particles arouses wide scientific and practical interest because of their possible use in various areas of optics, and in optoelectronics, in particular, as antireflection filters for lasers, for the generation of ultrashort and powerful laser pulses, and for devices of

Poster Session

fiber optic communications, ranging, and telecommunications. In our work the structural aspects of PbSnanoparticle formation in silicate glasses under different conditions of heat treatment are studied using smallangle neutron scattering. It is established that spherical nanoparticles with radiuses of 3.0 to 3.9 nm form in such glasses. As the duration of sample annealing increases, growth of the mean nanoparticle size is observed and their fractal dimensions change. The structural mechanisms for PbSnanoparticle formation in a glass matrix are discussed in the case of two stage temperature treatment.

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Effect of alkan-1-ols on the structure of DOPC model membrane

T. Kondela¹, J. Gallová¹, T. Hauss², N. Kučerka^{1,3}, O.I. Ivankov^{3,4,5}, P. Balgavy¹

¹Department of Physical Chemistry of Drugs, Faculty of Pharmacy, Comenius University, Bratislava, Slovakia

²Helmholtz Zentrum Berlin für Materialien und Energie, Berlin, Germany

³Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

⁴Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁵Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

kondela@fpharm.uniba.sk

We studied the effect of general anesthetics alkan-1-ols (CnOH, where n=10, 12, 14, 16 and 18 is the number of carbon atoms in molecule) on the structure of a model membrane system by small-angle neutron scattering (SANS) and diffraction (SAND). Extruded unilamellar liposomes for SANS measurements were prepared in excess of 100 % D₂O at the CnOH:DOPC=0.3 molar ratio. The data were evaluated by the Kratky-Porod plot $\ln[I(Q)Q^2]$ vs. Q^2 in the range of scattering vector Q corresponding to interval $0.001 \text{ \AA}^{-2} \leq Q^2 \leq 0.006 \text{ \AA}^{-2}$. The value of bilayer thickness parameter d_g has shown the trend in which the shorter alcohols (n=10, 12) decreased the thickness of DOPC bilayers while the longer ones (n=16) caused its increase. The results were corroborated with SAND measurements performed on the aligned multilayers that were utilized to eliminate the effect of bilayer curvature. Hydrated aligned fluid bilayers were prepared again from dioleoylphosphatidylcholine (DOPC) and samples at CnOH:DOPC=0.3 molar ratio were deposited on quartz plates by a „rock and roll method“. The samples were used for measurements at slightly dehydrated conditions (rel. humidity 98%, contrasts 8% , 20% and 50% D₂O) for improving the resolution of obtained results. From the scattering length density profile we found the similar trend to that of SANS results. Our results support the notion of the importance of lipid bilayer thickness and the possible mechanism of its modulation by the other membrane components, while this is unaffected by the bilayer geometry nor its hydration level.

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Transparent zirconia classes: synthesis, structure and optical properties

N.N. Gubanova^{1,2}, G.P. Kopitsa^{1,2}, A.E. Baranchikov³, V.K. Ivanov³

¹ Grebenshchikov Institute of Silicate Chemistry RAS, St.-Petersburg 199034, Russia

² Petersburg Nuclear Physics Institute NRC "Kurchatov Institute", Gatchina 188300, Russia,

³ Kurnakov Institute of General and Inorganic Chemistry RAS, Moscow, 119991, Russia
kopitsa@lms.pnpi.spb.ru

Transparent zirconia glasses were synthesized for the first time by sol-gel approach without the use of silicon compounds. Structure and properties of the materials obtained were analyzed using small-angle and ultra small-angle neutron scattering, small-angle X-ray scattering, low temperature nitrogen adsorption, X-ray diffraction analysis, scanning electron microscopy, thermal analysis and optical methods [1,2]. The synthetic approach involved the hydrolysis of zirconium propylate catalyzed by nitric¹ or acetic² acids.

All zirconia glasses are transparent X-ray amorphous materials possessing high specific surface areas (up to 250 m²/g). The structure of the glasses obtained using HNO₃ is characterized by three-level hierarchical fractal structure. The 1st level comprises primary ZrO₂ particles of $d_1 \approx 1$ nm size, which form fractal clusters having $d_2 \approx 24 \div 52$ nm size (2nd level). The 3rd level consists of relatively large ($d_3 \approx 2$ μ m) aggregates with diffuse surface.

The use of acetic acid as the hydrolysis catalyst leads to the formation of zirconia glasses with two-level hierarchical structure. The first level consists of primary ZrO₂ 1 nm size short-range ordered particles which form relatively large aggregates with diffuse surface (2nd level).

Both temperature of gelation and H₂O content in starting solution do not effect notably the structure of glasses.

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Human CysLT1 expression, purification, crystallization

A.P. Luginina¹, A.Yu. Gusach¹, A.V. Mishin¹, N.A. Vartanyan¹, R.O. Astashkin¹,
A.O. Bogorodskiy¹, M.M. Ergasheva¹, V.I. Borshchevskiy¹, V. Cherezov^{1,2}

¹ Moscow Institute of Physics and Technology, Dolgoprudnyi, Russia

² Bridge Institute, Departments of Chemistry and Physics & Astronomy, University of Southern California, Los Angeles, USA

Snurka88@gmail.com

CysLT1 is a human cysteinyl leukotriene receptor from class A GPCR superfamily. It is expressed in multiple tissues including spleen, peripheral blood leukocytes, smooth muscles of the lung, bronchial and intestinal tissues. Its sensitization activates process of bronchoconstriction, increased vascular permeability, mucus secretion and stimulates eosinophils migration [1]. Hence, CysLT1 is one of the major proteins involved in inflammation-related diseases including asthma and allergic rhinitis. CysLT1 antagonists such as Zafirlukast and Montelukast are widely used as add-ons in asthma treatment [2]. Solving CysLT1 structure should shed light on its functional activity and help with designing novel drugs with better functional selectivity and lower side effects.

The most successful method for GPCR structure determination is X-ray crystallography using crystals grown in lipidic cubic phase. Several milligrams of purified stable and monodisperse protein are typically required for crystallization trials. In this work various gene constructs of CysLT1 with apocytochrome b(562)RIL as a fusion partner [3] were designed and synthesized. Engineered protein constructs were expressed using baculovirus expression system in *Sf9* insect cells. Receptor purification and stabilization conditions, including buffer pH, salt concentration, purification steps, enzyme treatment, etc, were optimized. The best combinations of receptor constructs and ligands were selected based on monodispersity and thermal stability. Diffusion of the receptor in LCP at variety of conditions was analyzed with fluorescence recovery after photobleaching method, providing initial screening conditions for crystallization trials.

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Synthesis and Characterization of PEGylated Zinc Sulfide Nanopowders

A. Dumbrava¹, G. Podan², F. Moscalu³

¹ Department of Chemistry and Chemical Engineering, Ovidius University of Constanta, 124 Mamaia Blvd., Constanta 900527, Romania

² Electron Microscopy Laboratory, Ovidius University of Constanta, 124 Mamaia Blvd., Constanta 900527, Romania

³ Department of Physics and Electronics, Ovidius University of Constanta, 124 Mamaia Blvd., Constanta 900527, Romania

adumbrava@univ-ovidius.ro

Zinc sulfide (ZnS) is a wide direct band gap semiconductor, often used in technical fields like: electroluminescence, light-emitting diodes (LEDs), flat panel displays, sensors, lasers, solar cells, infrared windows, antimicrobial agent, biodevices, etc. [1-3].

Also, zinc sulfide is an efficient photocatalysts due to its fast production of electron-hole pairs under photoexcitation [4]. Its photocatalytic activity has been exhibited in the photodecomposition of some organic compounds [5], in the photocatalytic hydrogen production [6], etc. ZnS can be used in chemical industry and/or in environmental protection for the water treatment; e.g. in textile industry for decontamination of wastewater large quantities, which contain great amount of toxic dyestuff that have carcinogenic effects on human health. The photocatalytic degradation of dyes in the presence of semiconductors is an advanced oxidation process, resulting in the complete mineralization of most organic pollutants, with no further requirement for secondary disposal methods [7].

The PEGylation can be defined as a process of covalent and non-covalent attachment or amalgamation of polyethylene glycol (PEG) polymer chains to molecules and macrostructures. The PEGylation is often used for drugs, therapeutic proteins or vesicles [8], but it is also important in the synthesis of nanomaterials.

We compared the properties of PEGylated ZnS nanopowders, obtained by different synthesis routes. The morphology, optical and photocatalytic properties of PEGylated ZnS nanopowders were determined and reported to the pristine ZnS characteristics. The morphology of nanopowders was investigated by transmission electron microscopy. The photocatalytic properties of synthesized nanopowders were tested in the degradation of Congo red azo dye, demonstrating an enhancement of catalytic activity through capping zinc sulfide nanoparticles by the polymer, especially in the case of ZnS prepared in a non-aqueous medium, most probably because a strong interaction between the nanoparticles and the capping polymer.

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Small angle neutron scattering study of high-density polyethylene zirconium oxide nano composites

A.A. Nabiev^{1,2}, A.M. Maharramov², A.I. Kuklin¹, E.B. Asgerov^{1,3}

¹ Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russian Federation

² Institute of Radiation Problems, ANAS, 370143, Baku, Azerbaijan

³ National Centre for Nuclear Research, 370143, Baku, Azerbaijan

asifnebi@jinr.ru

The structure of High-density Polyethylene Zirconium Oxide Nano Composites (HDPE/ZrO₂) were studied by Small angle neutron scattering (SANS) at YUMO small angle time-of-flight diffractometer at the IBR-2 pulsed reactor (JINR, Dubna, Russia). HDPE/ZrO₂ composites contain different amounts (1%, 3%, 5%, 10%, 20%) of ZrO₂. Average nanoparticle size was 20-30 nm. Composite samples were obtained from the compound of homogeneous HDPE/ZrO₂ using thermal pressed method in temperature of 433 K and pressure of 15 MPa retaining 5 minutes, and then cooling in the water-ice system and liquid nitrogen. The samples were 5cm in diameter and 80-100 μ m in thickness. From SANS spectra Core Shell Ellipsoid Model was found for HDPE/ZrO₂ with SANS view program. The following results were obtained for ZrO₂ particles: the density- $d = 5.89 \text{ g/cm}^3$, the molar mass- $M = 123.218 \text{ g/mol}$, the scattering length- $b_{\text{ZrO}_2} = 1.876 \times 10^{-12} \text{ cm}$, the molecular volume- $V = 3.474 \times 10^{-23} \text{ cm}^3$ and the neutron scattering density- $\rho_{\text{ZrO}_2} = 5.4 \times 10^{10} \text{ cm}^{-2}$. The neutron scattering density and the scattering contrast for HDPE, however, were $\rho_{(\text{CH}_2)_n} = -0.34 \times 10^{10} \text{ cm}^{-2}$ and $\Delta\rho = 5.74 \times 10^{10} \text{ cm}^{-2}$ ($\Delta\rho = \rho_{\text{ZrO}_2} - \rho_{(\text{CH}_2)_n}$), consequently. Scattering vector (q) range was $0.005 < q < 0.39 \text{ nm}^{-1}$.

Magnetic nanoparticle properties studied with condensed matter methods and biochemical assays

L. Oprica¹, M. Andries², I. Bodale³, M. Balasoiu^{4,5}, D. Creanga²

¹ Faculty of Biology, Alexandru Ioan Cuza University, Iași, Romania

² Faculty of Physics, Alexandru Ioan Cuza University, Iași, Romania

³ University of Agricultural Sciences and Veterinary Medicine, Iași, Romania

⁴ Joint Institute for Nuclear Research, Dubna, Moscow Region, Russian Federation 141980

⁵ Horia Hulubei Institute of Physics and Nuclear Engineering, Bucharest, Romania

iasilacra@yahoo.com

Magnetic nanoparticles (MNPs) were synthesized by chemical route being stabilized in suspension by capping with organic acid. Nanometric size and superparamagnetic properties were evidenced with condensed matter methods: Scanning Electron Microscopy, Vibrating Sample Magnetometry, X-ray Diffraction. As methods of study the condensed matter interaction with living organisms the biochemical assays of antioxidant enzymes were applied. Cellulolytic fungi were chosen (Fig. 1) as biological material to evidence MNP impact on environment since engineered MNPs are known for some bioeffects in various organisms [1-3].

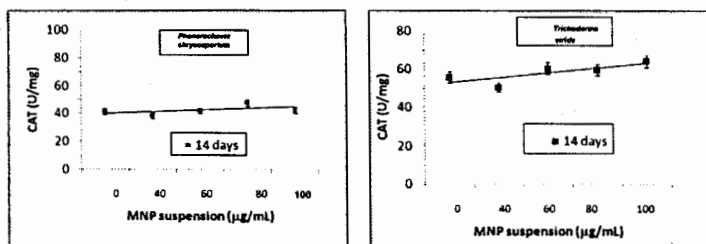


Fig. 1. Catalase (CAT) activity in the two test microorganisms

Catalytic action of metal ions released through MNP cellular digestion has generated reactive oxygen species, challenging fungi cells to intensify synthesis of antioxidant mechanisms as catalase enzyme to prevent other metabolic damages – CAT activity has increased. New investigation techniques are planned with SANS on the MNP powder and suspension.

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Mesoporous silica prepared using a pyridinium ionic liquid and studied by small angle scattering

A.-M. Putz¹, L. Almásy², A. Len², C. Ianăși¹, J. Pleštil³, C. Savii¹

¹ Institute of Chemistry Timisoara of Romanian Academy, Timisoara, Romania

² Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, Budapest, Hungary

³ Institute of Macromolecular Chemistry, Academy of Sciences, Prague, Czech Republic

Silica matrices have been prepared via acid catalysed sol-gel processing; both classic and sonocatalysed routes were used. As silica precursors, tetramethoxysilan (TMOS) and methyltrimethoxysilane (MTMS) were employed. Ionic liquid N-butyl-3-methylpyridinium tetrafluoroborate ([bmPy][BF₄]), a short alkyl chain IL, have been used in various proportions, aiming to catalyze the sol-gel reactions, and to influence the mesoporous silica materials properties, serving as pore template. Both small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) techniques were used in order to explore the dry gels microstructure evolution versus IL/Si molar ratios. In addition, the nitrogen adsorption-desorption isotherms allowed to obtain more information concerning materials morphology. The hypothesis that the ionic liquid co-solvent can play also catalyst's and/or pore forming agent's role was investigated both in classic and sono-catalysed systems.

The results show that basically the ionic liquid did play the role of catalyst, but it also affected the primary xerogel particles formation process, and it changed the porosity of the obtained materials. Ultrasound treatment resulted in some advantages. In comparison with xerogels, the prepared sonogels have showed increased pore diameter, bigger pore volumes but diminished surface areas. The ultrasound treatment resulted in microstructure adjustment on the level of the colloid particle aggregates. Compared the non-sonicated xerogels, at the highest IL content, the sonogel samples specifically exhibited almost double sized pore diameter [1,2]. The thermogravimetric and the differential thermal analyses were performed for both, the bare IL and the IL containing xerogels. It has been revealed that in confined geometry the decomposition of [bmPy][BF₄] starts at lower temperature compared to the case of the pure ionic liquid.

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SANS method study of surfactant mixture system nonionic+anionic in heavy water solutions

A. Rajewska^{1,2}, A.Kh. Islamov¹

¹ Joint Institute for Nuclear Research, LNP, 141980 Dubna, Russia

² National Centre for Nuclear Research, 05-400 Swierk-Otwock, Poland

aldonar@jinr.ru

The mixing of amphiphiles in water may lead to the formation of mixed micelles which often present new properties with respect to the pure component solutions [1, 2]. The mixture systems of classic surfactants TX-100+SDS (non-ionic+anionic)=(p-(1,1,3,3-tetramethyl) poly (oxyethylene))+ (sodium dodecyl sulphate) in water solutions were investigated at temperatures 30°, 50°, 70° for compositions 1:1, 2:1, 3:1 with the time-of-flight small-angle neutron scattering (TOF SANS) spectrometer ("YuMO") of the IBR-2 on pulsed neutron source [3] at FLNP, JINR in Dubna (Russia). Measurements have covered Q range from 8×10^{-3} to $0.4 \text{ \AA}^{-1}$. The SANS measurements of aqueous solutions of non-ionic/anionic surfactants have shown that micelles are formed in investigated solutions. From the measured dependence of the scattered intensity on the scattering angle, we derived the aggregation number of micelles at various compositions and the form and size of mixed micelles as a weak function of the mixing ratio between the two components and temperature. Experimental results were processed using the PCG Software 4.0 (Austria).

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**The fluxes of cold and thermal moderator at 4-th beam-line:
Monte-Carlo simulation and experiments**

A.D. Rogov¹, O.I. Ivankov^{1,2,3}, D.V. Soloviov^{1,2,3}, Yu.S. Kovalev^{1,2},
A.V. Rogachev^{1,2}, R.V. Erhan¹, A.I. Kuklin^{1,2}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

In this work the results of simulation and experimental data for cold and thermal moderator on 4-th beam-line of IBR-2 are presented. It was shown that ratio of flux of thermal to cold moderator in useful wavelength of neutron range for YuMO spectrometer is 3-4 times [1]. The results of experiments with same samples for cold and thermal moderator are compared. The possibility to modernize and adaptation of instrument to cold moderator which is planned to appear in 2019 are discussed.:

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Properties of the magnetic nanoparticles of gallium ferrites and ferrofluids

K. Rečko¹, J. Waliszewski¹, U. Klekotka², D. Satuła¹, F. Damay³,
M. Biernacka¹, M. Balasoiu⁴, K. Szymański¹

¹ Faculty of Physics, University of Białystok, K. Ciołkowskiego 1L, 15-245 Białystok, Poland

² Institute of Chemistry, University of Białystok, K. Ciołkowskiego 1K, 15-245 Białystok, Poland

³ Laboratoire Léon Brillouin, UMR12 CEA-CNRS, Bât. 563 CEA Saclay, 91191 Gif sur Yvette Cedex, France

⁴ The Frank Laboratory of Neutron Physics, JINR, Joliot-Curie str. 6, Dubna, Moscow reg., Russia, 141980

k.recko@uwb.edu.pl

In this case of gallium ferrites ($\text{Ga}_x\text{Fe}_{2-x}\text{O}_3$) we are talking about a kind of novel functional materials, which possess two switchable states such as polarization and magnetization [1]. Ferromagnetic and ferroelectric orders coexist in these systems and their physical behavior can be modulated by magnetic or electric field, respectively [2]. Magnetic properties of the system are strongly correlated with the nonequivalent distribution of cations Fe^{3+} and Ga^{3+} in crystalline sublattices (see Fig. 1), whereas anions O^{2-} are important because of the type of coordination of the cation and the mechanisms of exchange magnetic interactions. According to previous [3-4] and presented herein paper neutron data the commensurability of the system is fulfilled. While the collinearity of the system is broken. The neutron data disclosed antiferromagnetic order of

iron magnetic moments along c axis with a small tilting angle in the ac plane. Thereby the spontaneous electric polarization is expected along the b axis.

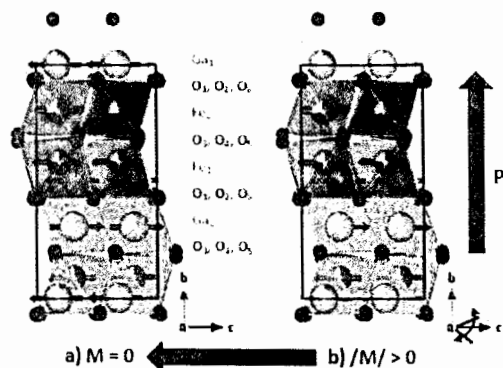


Fig. 1. Low temperature projection view of the crystal structure of (a) totally disordered and (b) typically ordered GaFeO_3 along the a axis.

The stable and well dispersed in a solution nanoparticles of magnetite (Fe_3O_4) guarantee as a specific feature the magnetic control of their physical parameters. Nanoparticles of ferrofluids have same unique properties, for example the so-called lock superparamagnetic field density temperature or the active surface [5]. Noteworthy, the magnetic properties strongly depend on the size and the shape of

nanoparticles [6]. A much greater effective magnetic moment resulting from coupling of a number of nuclear spins is observed.

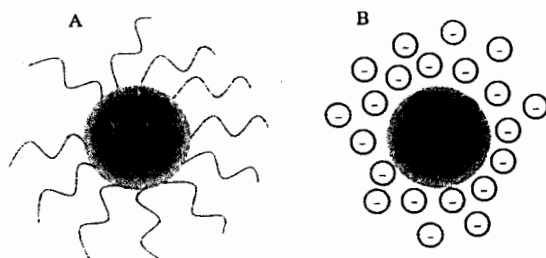


Fig. 2 Steric (A) and electrostatic (B) stabilization of magnetite nanoparticles.

Ferrofluids are two-phase systems, where one is solid (nanoparticles), and other is liquid. They have been found to possess very interesting

thermophysical properties e.g. thermal conductivity, thermal diffusivity, viscosity or convective heat transfer coefficient. Therefore, particles dispersed in fluids can find great applications potential in many fields [7]. One of the major issue of preparation of ferrofluids is their stability, because especially magnetic nanoparticles tend to agglomerate due to high magnetic forces. There are two ways to enhance stability of the ferrofluids. First of all, it can be achieved by coating of nanoparticles with surfactant, to produce entropic repulsion (see Fig. 2), or with charging of the particles surface, thereby an electrostatic repulsion is observed. Obviously, the use of magnetic nanoparticles requires proper control of their growth. As the complementary methods for condensed matter research the elastic X-ray, neutron diffraction techniques and Mössbauer Spectroscopy as well as DC – magnetization measurements results are presented.

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Lipidic membranes structural conformations in aqueous solutions from SAXS and SANS comparative analysis

M.I. Rulev^{1,2}, D.V. Zabelskii³, A.V. Vlasov³, D.V. Soloviov^{1,3,4}, O.I. Ivankov^{1,3,4}, Yu.L. Ryzhykau³, E.V. Zinovev³, V.I. Gordeliy^{1,3,5,6}, A.I. Kuklin^{1,3}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Lomonosov Moscow State University, Moscow, Russia

³ Moscow Institute of Physics and Technology, Dolgoprudny, Russia

⁴ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁵ Institute of Structural Biology, Grenoble, France

⁶ IBS-5, Forschungszentrum Juelich, Germany

kuklin@nf.jinr.ru, rulevmaksim@gmail.com

Investigation of lipidic membranes near the phase transition point has a significant importance not only for theoretical findings, but also from biological point of view [1]. DPPC aqueous solution are known to have the main phase transition temperature point near 41°C [2]. Structural conformations of periodicity or lipidic membranes thicknesses occur in much wider temperature range. In this work SAXS and SANS data are represented and compared. In addition, densitometry data were involved for more detailed analysis. Densitometry data add information about the phase-transition point that is usually taken as the main one. In particular, the phase transition temperatures differ with 0,35°C in water and heavy water solutions. SANS measurements were done on small-angle spectrometer YuMO [3] (IBR-2, JINR, Dubna, Russia). SAXS were done on Rigaku spectrometer (MIPT, Dolgoprudny, Russia) [4]. We found that DPPC structural conformations start at near 38 °C and finish near 48 °C. Winter and coauthors [2] the temperature range 34–42 °C is called “ripple-phase”. Dependences of the periodicity as the function of temperature allowed calculating phase-transition temperatures. We have obtained that the periodicity values are different when providing SAXS or SANS measurements. The SAXS results show a wider transition area and a lower maxima values of periodicity than the SANS results. Reasons of discrepancies in methods and possible lipidic phase states are discussed.

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Investigations of the phase transition of DPPC MLVs co-dispersed in water solution with potassium chloride

M.I. Rulev^{1,3}, O.I. Ivankov^{1,2,4}, D.V. Soloviov^{1,2,4}, D.V. Zabelskii², A.V. Vlasov², Yu.L. Ryzhykau², E.V. Zinovev², N. Kučerka¹, V.I. Gordeliy^{1,2,5,6}, A.I. Kuklin^{1,2}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, Dolgoprudny, Russia

³ Lomonosov Moscow State University, Moscow, Russia

⁴ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁵ Institute of Structural Biology, Grenoble, France

⁶ IBS-5, Forschungszentrum Juelich, Germany

rulevmaksim@gmail.com, kuklin@nf.jinr.ru

In this work we present results of SANS and SAXS studies of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) in heavy water solution with potassium ions. Some authors claim the adding of different metal ions into solution increases the main phase transition temperature [1,2].

We used commercially available lipids produced by Sigma-Aldrich. Structural changes of lipids were studied on the spectrometer YuMO, IBR-2 at JINR, Dubna, Russia[3], and Rigaku at MIPT, Dolgoprudny, Russia[4]. The temperature induced changes to the lipid density were investigated by densimetry method on instrument AntonPaar DMA 5000M at JINR, Dubna, Russia.

The gel – liquid phase transition for DPPC dispersed in heavy water at low concentrations is known to go through the ripple phase [5]. With the help of SAXS and SANS methods we found that ripple phase formation starts at near 36°C and is not affected when changing the concentration of potassium ions in solution. Densimetry data revealed the phase transition temperature of 41,7°C that is in a excellent agreement with literature. The comparison with other authors works is made. Results of densimetry and SAS data treatment are discussed.

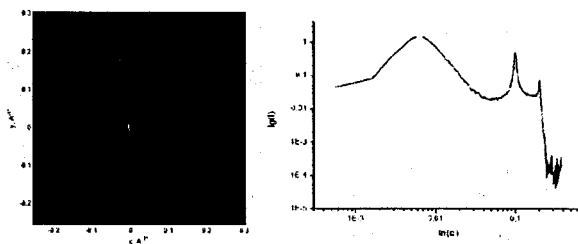


Fig.1. Typical 2D SAXS pattern (left) and Intensity of q (right) of DPPC MLVs co-dispersed in water solution with potassium chloride.

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About the possibilities of Small Angle Scattering method: applications to nanodiscs structure studies

Yu.L. Ryzhykau¹, M.Yu. Nikolaev^{1,2}, D.V. Soloviov^{1,3,4}, O.I. Ivankov^{1,3,4}, Yu.S. Kovalev^{1,3},
T.N. Murugova^{1,3}, E.V. Zinoviev^{1,3}, A.V. Vlasov¹, A.V. Rogachev^{1,3}, V.I. Borshchevskiy¹,
V.I. Gordeliy^{1,3,5,6}, A.I. Kuklin^{1,3}

¹ Moscow Institute of Physics and Technology (State University), Dolgoprudnyi, Russia

² École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

³ Joint Institute for Nuclear Research, Dubna, Russia

⁴ Institute for Safety Problems of Nuclear Power Plants, Kyiv, Ukraine

⁵ Institute of Complex Systems (ICS), ICS-5: Molecular Biophysics, Research Centre Juelich, Juelich, Germany

⁶ Institute of Structural Biology J.P.Ebel, Grenoble, France

rizhikov@phystech.edu

Small Angle Scattering (SAS) is a powerful method for investigation of wide range of objects: large-scale structures, defects in materials, colloids, polymers, proteins, biological membranes, viruses, macromolecules and so on [1]. In this work are presented examples of SAS method possibilities for structure studying of nanodiscs.

Nanodisc (ND) is a synthetic membrane mimicking system, which is composed of a fragment of phospholipid bilayer and peptides [2] or two Membrane Scaffold Proteins (MSP) [3]. NDs have applications for functional and structural investigation of membrane proteins [4-7].

Some characteristics of ND are monodispersity (in case of MSP), symmetry, sizes along the different axis have the same order, it is complex multiphase system. Thus ND is a model object for SAS method possibilities demonstration.

In this work we show results of different SAS applications for structural studies of ND:

1) The scattering intensity at zero angle and radius of gyration (R_g) could be calculated from SAS curve using Guinier approximation [1, 8]. It was done for series of temperature points. Obtained R_g temperature dependence was used for structural phase transition investigation of lipids DMPC and DPPC included in ND [9].

2) Peptide nanodisc was modeled as a set of cylindrical peptide belt and cylindrical fragment of lipid bilayer, which was modeled set of two components: hydrophobic and hydrophilic layers. All this parts assumed to have constant electron density. Patterson function ($P(r)$) [1] for this model of ND was calculated and analyzed. Using comparison with $P(r)$ calculated from experimental SAXS data it was proved that peptides and lipids really form nanodiscs [10].

3) Model of ND from p. 2 was used for fitting of experimental SAXS curve [11]. Optimal parameters of ND model were found (without polydispersity analysis).

4) The contrast variation method [12-13], applied in a SANS experiment, was used to obtain information about average density of coherent scattering length and volume of ND (prepared from MSP), parameters of elliptical cylinder structure of lipid bilayer and MSP belt. Also using program DAMMIN [14] were obtained low-resolution structures of lipid bilayer and MSP belt and low-resolution structure of "shape" of ND (assuming it to be homogeneous particle) [1, 13].

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Monte Carlo simulation of SESANS experiment with time-gradient magnetic fields

V.V. Sadilov^{1,2}, V.I. Bodnarchuk¹, S.A. Manoshin¹, R.V. Erhan¹, A. Ioffe³

¹ Joint Institute for Nuclear Research, Frank Laboratory of Neutron Physics, Joliot Curie 6, 141980 Dubna, Moscow region, Russia

² Lomonosov Moscow State University, Faculty of Physics, Leninskiye Gory 1, 119991 Moscow, Russia

³ Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science-Outstation Garching, Lichtenbergstr. 1, 85747 Garching, Germany
sadilov.valentin@mail.ru

A new neutron spin-echo method based on the use of time-gradient magnetic field has recently been proposed. This method is one of the variants of neutron spin-echo technique that is applied to pulsed neutron source such as being built now at ESS in Lund. SESANS instrument that applicate such technique is being developed in Dubna at the IBR-2 at the present time. This study presents the operational modes of a virtual SESANS instrument built by using the simulation package VITESS with parameters of developing machine. In addition, the issue of resolution improving applying scattered beam collimation was considered. The sectoral and rectangular collimators in the SESANS method with time-gradient magnetic fields are considered by means of Monte-Carlo simulations in VITESS package. It is shown, that the use of a sectoral collimator improves resolution and time of measurement in spite of the excluded part of scattered neutrons.

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The investigation of the structure of bicelles by small-angle scattering method

D.V. Seliverstova^{1,2}, O.I. Ivankov^{2,3,4}, T.N. Murugova^{2,3}, D.V. Soloviov^{2,3,4},
A.I. Kuklin^{2,3}, V.I. Gordeliy^{2,3}

¹"Dubna" University, Dubna, Russia

²Joint Institute for Nuclear Research, Dubna, Russia

³Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

⁴Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

seliwyorstova.daria@yandex.ru

The results of the small-angle X-ray (SAXS) and neutron (SANS) scattering experiments on bicellar systems are presented. The main goal of the experiments is to investigate the changes of the bicellar structural parameters during the crystallization of membrane proteins. The measurements were carried out on the samples with the molar ratio of DMPC/CHAPSO = 2.7, with different concentrations of the lipids, buffer composition at different temperatures.

The measurements were carried out on the Rigaku spectrometer (MIPT, Dolgoprudny) and YuMO spectrometer (JINR, Dubna).

The scattering intensities depending on the scattering vector were obtained during the experiments. The experimental scattering curves were approximated by the bicelles and cylinder models using the SASView program package without taking into account the interaction between the bicelles in solution.

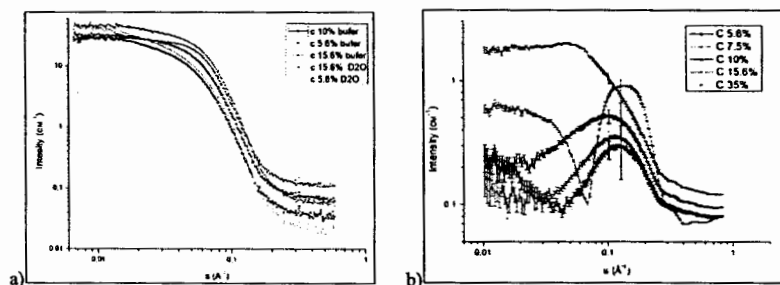


Fig.1 The graphs of the scattering intensity (I) from the scattering vector (s) for (a) SANS and (b) SAXS depending on the different concentrations of lipids (C) at a temperature 20°C .

Curves SAXS and SANS drastically differ for the same samples that are associated with the heterogeneity of the system.

Poster Session

The experiments showed the changes of the structural parameters of the bicelles with the changes of the lipid concentration, buffer composition and time of the stabilization of the solution.

The work was supported by the Ministry of Education and Science

The authors are grateful the program "5 Top 100"

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The effect of thermal treatment on the atomic structure of PtCu core-shell nanoparticles in PtCu/C electrocatalysts

D.B. Shemet, V.V. Pryadchenko, V.V. Srabionyan, S.B. Belenov,
L.A. Avakyan, V.E. Guterman, L.A. Bugaev

Southern Federal University, Rostov-on-Don, Russia
Shemetdabo@mail.ru

Composite materials containing noble metal nanoparticles are extensively synthesized and studied because they exhibit valuable functional characteristics, being highly efficient catalysts towards oxygen electroreduction and hydrogen electrooxidation [1,2]. Nanocatalysts PtCu/C with core-shell structure of PtCu nanoparticles were synthesized by the method of simultaneous chemical reduction of Cu^{2+} and Pt(IV) in carbon suspension, prepared on the basis of ethylene glycol–water solvent. The characterization of atomic structure of as prepared PtCu nanoparticles and obtained after thermal treatment at different temperatures in range between 200 °C and 350 °C, was performed by Pt L_{3-} and Cu K -edge extended X-ray absorption fine structure (EXAFS) using the technique for determining local structure parameters of the absorbing atoms, which have the nearest surrounding consisting of Pt and Cu atoms [3,4]. The spectra were measured at the μSpot beamline of the BESSY-II Synchrotron Radiation Facility (Berlin, Germany).

EXAFS spectroscopy is one of efficient methods for the study of nanoparticles because of its sensitivity to local atomic structure and composition, high spatial resolution and applicability in absence of long-range order. Meanwhile, EXAFS derived values of parameters for the nearest neighbors of absorbing atoms in bimetallic nanoparticles enable to make only indirect conclusions on the atomic structure of the studied nanocatalysts. To determine the relationship between the synthesis or treatment conditions – atomic structure – electrochemical performances of these materials, it is necessary to visualize the character of components distribution over the volume of nanoparticle, in correspondence with the values of structural parameters derived from EXAFS.

3D modeling of the atomic structure of bimetallic nanoparticles in PtCu/C electrocatalysts was performed by simulations of the atomic clusters, which correspond to the values of the local atomic structure of Pt and Cu atoms derived from EXAFS [5]. These models enabled to reveal the relationship between temperatures of thermal treatments and components distributions over the volume of PtCu nanoparticles in the studied electrocatalysts.

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Modernization of the control motors and sample environment system of YuMO spectrometer at IBR-2M

**A.P. Sirotin¹, A.S. Kirilov¹, T.B. Petukhova¹, D.V. Soloviov^{1,2,3},
O.I. Ivankov^{1,2,3}, A.I. Kuklin^{1,2}**

¹ Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

sirota@nf.jinr.ru

Currently, many spectrometers at IBR-2M conducted a comprehensive upgrade of control systems and management experimental installations.

This paper presents the basic approaches to the construction of systems of control and management of experimental facilities at the IBR-2M.

As an example, the control and management system of the experimental setup YuMO 4 channel IBR-2.

To connect the spectrometer hardware to PC using the USB interface. Adapters are used in the management and control system:

- USB-RS485- for connecting control systems.
- RS485-SSI - to connect the position sensors of the actuators to the RS485 line.
- RS485-RS232 - for connection of devices with an RS232 interface to the RS485 line.

Control system of executive mechanisms is based on interface RS 485. AC4 USB-RS485 adapter (OWEN) communicates with a PC via the RS485 group of up to 32 stepper motor controllers OSM42 or OSM88 (Onitex) by RS485 link.

Data acquisition system with sensors and is based on the RS485 interface. AC4 USB-RS485 adapter (OWEN) communicates with a PC via the RS485 group of up to 32 controllers LIR915 (SSI-to-RS485, «SKB IS»). Controllers LIR915 used for reading information from the absolute multi-turn angular sensors MCD (FRABA Inc.).

To connect devices with RS232 interface to the RS485 line. used RS485-RS232 converters.

Small-angle neutron scattering study of phase transitions of mixed lipid membranes in water solution

A.Y. Sluchevsky^{1,2}, D.V. Soloviov², M.I. Rulev^{1,2}, A.I. Kuklin²

¹ Lomonosov Moscow State University, Moscow, Russia

² Joint Institute for Nuclear Research, Dubna, Russia

tommyjkee@gmail.com

Each living cell is surrounded by a membrane, which provides inside the cell the necessary "climate" plays an active role in maintaining its activity, controls the flow of substances and ions into the cell and out of it. Membrane is the most important part and cellular components, and therefore the cell membrane plays a key role in biological processes. Lipid membranes are a good model for numerous biophysical studies.

Studies of the physical and physico-chemical aspects of phase transitions in membranes (real biological and model lipid) has been going for many years [1-2]. This interest is due both to the biological importance of the membranes and their promising applications (such as sensors, transducers, filters), and with the fundamental physical issues related to phase transitions, fluctuations, and dynamics of complex systems.

The phase transition temperature point is dependent on the variation of some parameters such as pressure. A pressure is a particularly interesting case, as the number of living organisms is in extreme external conditions - high pressures and temperatures as well as mixture of lipids [1,3].

In present work we study of multilayer membranes (MLV) of lipid mixtures by the method of small-angle x-ray scattering and small-angle neutron scattering. Biological cell membrane is composed of many lipids, therefore, to create a model membrane were taken two lipids with very different temperature points of the main phase transition.

Using the methods of SAS and densimetry one we study changes of structure and density of mixture lipid as the temperature function. SANS measurements were performed on small-angle spectrometer YuMO [4] (IBR-2, JINR, Dubna, Russia), SAXS measurement on the spectrometer Rigaku (MIPT, Dolgoprudny, Russia) [5].

The results of research of phase transitions of lipid membranes and mixtures depending on pressure and temperature are presented. It is known that at low mass ratios in aqueous solutions of DPPC is present in 3 main phases: 35°C when a phase transition occurs from a gel phase to ripple phase, and at about 41°C from ripple-phase to fluid phase.

It has been established that the formation of the ripple phase starts at temperatures of about 36°C and remains unchanged for different concentrations with the addition of POPC lipid. The

transition to the ripple phase is carried out with a considerably smaller change of the period of recurrence compared with pure DPPC solution. Densimetry data obtained on the densimeter AntonPaar 5000M, complementary information about the phase transition point, is taken as the point of the main phase transition. We are compared our results with another data reported. The reasons for the differences are discussed.

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**Structural morphology of *Gluconacetobacter xylinus* cellulose,
and of organo-inorganic composite materials on its base**

R. Smyslov^{1,2}, G. Kopitsa², Yu. Gorshkova³, O. Ivankov³, K. Ezdakova²,
Yu. Chetverikov², A. Bugrov^{1,4}, A. Zavialova⁴, A. Khripunov¹, A. Tkachenko⁵,
V. Haramus⁶, B. Angelov⁷, V. Pipich⁸, N. Szekely⁸

¹ Institute of macromolecular compounds, RAS, St. Petersburg, Russia

² Petersburg Nuclear Physics Institute, National Research Center "Kurchatov Institute", Gatchina, Leningrad district, Russia.

³ The Joint Institute for Nuclear Research, Dubna, Russia

⁴ Saint Petersburg Electrotechnical University "LETI", St. Petersburg, Russia

⁵ Saint Petersburg State University, St. Petersburg, Russia

⁶ Laboratory EMBL, EMBL HAMBURG, DESY, Hamburg, Germany

⁷ Institute of Physics, ELI Beamlines, Academy of Sciences of the Czech Republic, Praha, Czech republic

⁸ JCNS, Forschungszentrum Juelich GmbH, Outstation at MLZ, Garching, Germany

urs@mail.macro.ru

The goal of material sciences is to obtain new composites with unique properties which are necessary for medicine (e.g., radiological treatments and photodynamic therapy of cancer), optoelectronics, constructional materials, protective clothing. In this study, we obtained composites based on the cellulosic scaffold that is from *Gluconacetobacter xylinus* cellulose (GxC) nanogel film preliminary disintegrated and air-dried. As functional components ZrO₂ nanoparticles were used, which are excellent optical matrix for Ln³⁺ ions due to suitable band gap, high refractive index, photochemical stability and transparency in a wide spectral range. The desired "red" and near-infrared optical luminescence ranges might be achieved by incorporating Eu, Er and Yb ions in zirconia. Metal-polymer complexes based on water-soluble polymer ligands with Ln³⁺ ions can also be used for such purpose. The morphology and structural properties of the biocompatible GxC matrix were varied by physicochemical treatment (disintegration degree, drying method).

Using complementary methods (small angle X-ray scattering, small and very small angle neutron scattering, low temperature nitrogen adsorption, wide-angle X-ray diffraction, as well as electron microscopy), it was found that the GxC composites obtained have multilevel fractal structure. The resulting composites were also studied by luminescence spectroscopy. The luminescent properties of composites depend on the presence of ZrO₂ nanoparticles and the employing type of Ln³⁺ ions. The results are important in the context of nanotechnologies for regenerative medicine, lightweight materials and optoelectronics.

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SAS program: current status and future

A.G. Soloviev¹, O.I. Ivankov^{1,2,3}, D.V. Soloviev^{1,2,3}, A.V. Rogachev^{1,2},
Yu.S. Kovalev^{1,2}, T.M. Solovjeva^{1,2}, A.I. Kuklin^{1,2}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine
soloviev@jinr.ru

The current version of raw spectrum data treatment program for YuMO spectrometer is available in [1,2] and is mainly described in [3,4]. Program is adapted to the specific feature of spectrometer, namely: two detector system [5], Vn-standard in front of each detector, direct beam geometry, good resolution, high flux, many configurations of experiments, several types of normalization. Main changes of described program package for YuMO spectrometer data treatment are related to adaptation for two detector system. The algorithms are corrected and detailed in comparison with previous version [3,4]. Due to new data format and another changes (for example channel range for each wire) in program the possibilities of the program are increased. More user-friendly interface has been achieved. The modification of the program was realized in several stages. The investigations for the time channels width corrections due to the samples with low scattering was performed. These changes are necessary for future data treatment of position sensitive detector as well.

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Corporate information system for development of SANS software

A.V. Rogachev^{1,2}, A.G. Soloviev¹, O.I. Ivankov^{1,2,3},
D.V. Soloviev^{1,2,3}, T.M. Solovjeva¹, A.I. Kuklin^{1,2}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, MIPT, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

Continuous updating of the information technologies, significant increasing the number of users of small-angle neutron scattering spectrometer, needing of interaction of collectives with various specialization, and also systematic change of research technique, the controlled and operated parameters structure, have demanded creating the multipurpose information system capable to keep continuity of earlier created code at change of a research method and a the equipment configuration.

The developed integration decision represent the set of the technologies allowing in limited terms and with the minimum expenses to provide sharing functioning of information systems modules and applications, untied at the technological level.

Experimental data from the YuMO spectrometer[1] are arrived in the continuous mode to the DATA center where are stored in as binary or XML files.

The control version system Git[2] is intended to automate work with files history, to provide changes monitoring, data synchronization and to organize the protected storage for a program code.

The completely customized by issue-tracking project management system JIRA[3] has been applied for the most effective work on improvement of the software, the registration of the changes made to program structure.

Development the Internet does web browsers by the dominating interface type for access to contents, applications and systems worldwide. Creation of information system is conducted taking into account this tendency. The website of the YuMO spectrometer is designed taking into account possible extensibility.

In general, using of corporate information system brings an obvious positive effect. It helps to operate requirements to the software, provides modification simplicity and support of the software, provides qualitative feedback, allows to document better errors, remarks and wishes, quickly to react to these wishes.

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Fractal analysis of CoFe_2O_4 /lauric acid/DDS-Na/ H_2O ferrofluid from TEM and SANS measurements

M. Balasoiu^{1,2}, O.I. Ivankov^{1,3}, C. Stan⁴, D. Buzatu⁴, C.P. Cristescu⁴

¹ Joint Institute for Nuclear Research, 141980, Dubna, Russia

² "Horia Hulubei" National Institute of Physics and Engineering, P.O. Box.MG-6, Bucharest, Romania

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁴ "Politehnica" University of Bucharest, Department of Physics, Faculty of Applied Sciences, Romania
cstan@physics.pub.ro

Cobalt ferrite nanoparticles (CoFe_2O_4) have been extensively studied in the last decades due to their remarkable magnetic properties that open new possibilities for technological and medical applications.

In the present study microstructural system characterization is performed by fractal analysis on the results of small angle neutron scattering (SANS) and transmission electron microscopy (TEM) investigations on a new CoFe_2O_4 /lauric acid/DDC-Na/ H_2O ferrofluid.

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

SANS measurements were carried out using the YUMO instrument installed at IBR-2 high pulsed reactor (JINR, Dubna, Russia), equipped with a two- detector system. The range of the scattering vector Q was $0.006 \text{ \AA}^{-1} < Q < 0.3 \text{ \AA}^{-1}$. 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} .

SANS experimental curves of 3% CoFe_2O_4 /lauric acid/DDC-Na/ H_2O particle vol. concentration ferrofluid samples and the corresponding TEM image are shown in Fig.1.

From SANS experimental curve of 3% CoFe_2O_4 /lauric acid/DDS-Na/ H_2O particle vol. concentration ferrofluid samples, the slope of the linear part in the intermediate region is -3.71 ± 0.04 , demonstrating that the scattering objects are in a first order approximation surface fractals with main fractal dimensions $D_s = 2.29$.

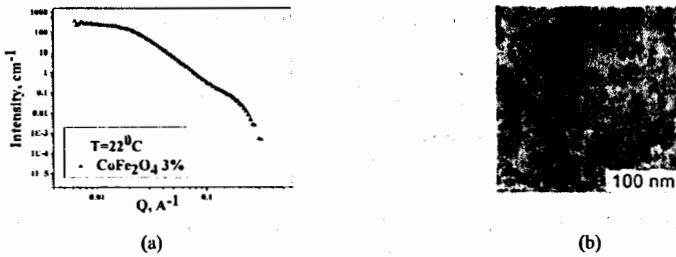


Fig.1: (a) SANS experimental curves of 3% CoFe₂O₄/lauric acid/DDS-Na/H₂O particle vol. concentration ferrofluid samples and (b) the corresponding TEM image [2].

This dimension can be found in the multifractal spectrum (Fig.2a) and in plot of the generalized dimension (Fig.2b) computed from TEM images (using the standard box-counting method [3]), corresponding to $q = -2.53$ which is specific to small fluctuations values from the mean.

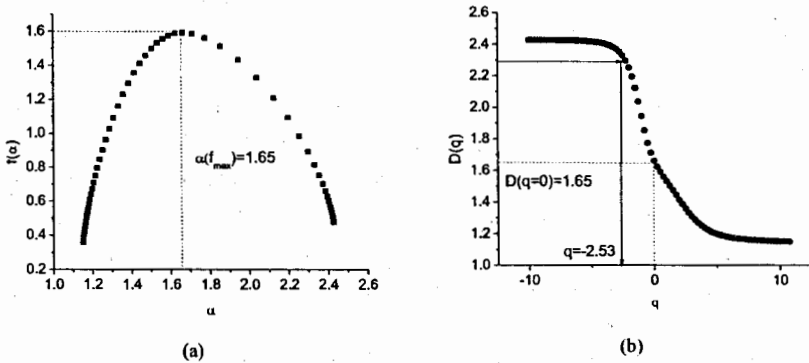


Fig.2: Multifractal spectra (a) and the generalized dimension for the TEM image (b)

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Self-assembly of endofullerenol-water systems

M.V. Suyasova¹, Yu.V. Kulvelis¹, V.T. Lebedev¹,
A.A. Szhogina¹, V.P. Sedov, A.I. Kuklin²

¹ Petersburg Nuclear Physics Institute, 188300, Gatchina, Russia

² Joint Institute for Nuclear Research, 141980, Dubna, Russia

marinasuyasova@pnpi.spb.ru

The biomedical applications of endometallofullerenes makes very important a comprehensive analysis of their water-soluble forms behavior in aqueous solutions under particular conditions (temperature, concentration) existing in living organisms. Rare earth (RE) elements encapsulated in metallofullerenes are the most important family in the endohedral fullerenes, due to their potential applications. They have been proposed for applications in many fields including biomedical uses. Extensive applications come from properties of a tremendous number of their derivatives that can be designed according to the practical demands and produced by chemical/physical modifications of carbon cages. Due to unpaired electrons in the metallic atom of the rare earth element, their application in magnetic resonance imaging (MRI) is an intriguing topic.

In particular, it is necessary to know the peculiarities of molecular interactions of fullerenols $\text{Re}@\text{C}_{82}(\text{OH})_x$ ($X \sim 38-40$) in comparison with $\text{Gd}@\text{C}_{82}(\text{OH})_x$ ($X \sim 30$) [1-3] in aqueous media and to recognize the trends of their self-assembly since these substances are considered as advanced agents to achieve high contrast in MRI when these substances are administrated in tissues for diagnostics tests [4]. The study of these objects is relevant, in particular because of the dependence of the relaxation rate from gadofullerenols aggregation in solutions. In the research [5] water-soluble multi-hydroxyl some lanthanoid (La, Ce, Gd, Dy, and Er) endohedral metallofullerenes ($\text{M}@\text{C}_{82}(\text{OH})_x$) have been characterized for the use of MRI contrast agents. Also interesting objects are endofullerenes with samarium, europium, terbium, thulium, and that exhibit the ability to luminescence.

The aim of the investigation was the study of supramolecular structures of fullerenes' $\text{M}@\text{C}_{82}(\text{OH})_x$ in aqueous solutions when their content varies in the range $C = 1 - 3 \%$. Modeling aggregation of different fullerenes, their water-soluble derivatives, as well as the effect of the encapsulated metal atom on the structure and formation of clusters is an important task.

We have measured two series ($\text{pH} = 3; 7$) of aqueous solutions with concentrations 1,5% of $\text{Re}@\text{C}_{82}(\text{OH})_x$ fullerenols ($\text{Re} = \text{Pr}, \text{Sm}, \text{Eu}, \text{Gd}, \text{Tb}, \text{Dy}, \text{Ho}, \text{Tm}$) at 20°C and 37°C to perform conditions of storage at room temperature and application inside living organisms. Solutions with

pH~3 are fullerlenols in pure distilled water, pH~7 was achieved in phosphate buffer. Measured curves at YuMO facility at 20°C are shown at fig. 1a. The curves demonstrate globular objects having a sharp border (slope of SANS-curves ~ 4) that corresponds well to preliminary results obtained at PNPI, Gatchina. The rise at higher q may be due to individual fullerlenol molecules existing in solutions. Therefore, using of stabilized (phosphate buffer) components allow achieving very stable aggregates of fullerenes with selected number from rare earth elements. Fig. 1b shows recovered correlation functions in spherical representation, demonstrating correlations in the spherical layers at the radius R around any particle and giving information about the presence of different sizes of aggregates.

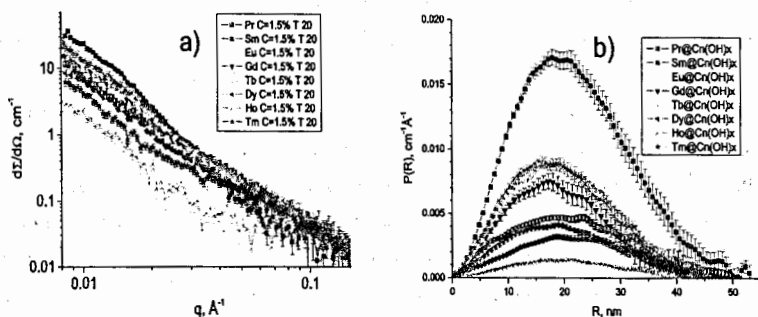


Fig. 1. SANS of fullerlenols in aqueous solutions (pH=3) a) cross sections; b) correlation functions.

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Small-angle scattering sheds light on dimerization mechanism of iron-regulating protein apoferritin

A.V. Vlasov¹, Yu.L. Ryzhykau¹, E.V. Zinoviev¹, D.V. Soloviov^{1,2,3}, O.I. Ivankov^{1,2,3},
P.K. Utrobin¹, A.V. Mishin¹, V.I. Gordeliy^{1,2,4,5}, V.I. Borshevskiy¹, A.I. Kuklin^{1,2}

¹ Laboratory for advanced studies of membrane proteins, Moscow Institute of Physics and Technology, Dolgoprudny, Russia

² Joint Institute for Nuclear Research, Dubna, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁴ Institute of Complex Systems (ICS-6), Juelich, Germany

⁵ Institut de Biologie Structurale J.-P. Ebel, Grenoble, France

alexander.iv.kuklin@gmail.com

Apoferritin dimerization in salt-aqueous solutions was investigated by means of size exclusion chromatography (SEC) and small-angle X-ray scattering (SAXS). Low-resolution structures and main integral invariants could be easily obtained from SAXS-curves [1]. We showed that apoferritin solution usually has a significant part of dimers and other multimeric protein aggregates and it has to be taken into account for more accurate SAS data analysis [2].

In this work we found the correlation between effective gyration radius of apoferritin and the number of the molecules that have formed aggregates. For aqueous apoferritin solution the salt screening was done with gradient of sodium chloride (NaCl) and the SAS pictures with corresponding low-resolution structures are presented. We showed that the influence of structural factor decreases and the protein aggregation increases when adding more NaCl. The nature of this process is being discussed.

SAXS was done on BM29 beamline in ESRF, Grenoble, France. Data collection, processing and analysis were performed automatically by software specifically developed for beamline – BsxCuBE [3].

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Authors list

Keynote Speakers

Burzo E. _____	16	Stuhrmann H.B. _____	22
Katsaras J. _____	18	Teixeira J. _____	24
Michels A. _____	19	Zaccai N.R. _____	25
Ozerin A.N. _____	21		

Invited Speakers

Arzumanyan G.M. _____	28	Kopcansky P. _____	38
Avdeev M.V. _____	29	Kučerka N. _____	40
Cser L. _____	31	Lebedev V.T. _____	41
Gille W. _____	32	Runov V.V. _____	43
Iacomini F. _____	34	Uhríková D. _____	44
Isaev-Ivanov V. _____	36	Vladoiu R. _____	45
Jestin J. _____	37	Volkov V.V. _____	48

Contributed Talks

Creanga D. _____	51	Pribora V. _____	62
Ivankov O.I. _____	52	Shibaev A.V. _____	64
Kulvelis Yu.V. _____	53	Shiryaev A.A. _____	66
Larichev Yu.L. _____	55	Shvetsov A.V. _____	68
Lebedev D.V. _____	56	Soloviov D.V. _____	52
Molchanov V.S., _____	57	Tomchuk O.V. _____	70
Motovilov K.A. _____	59	Zhigunov A.N. _____	72
Ostrovsky M.A. _____	61		

Authors List

Poster Session

Anghel L. _____	76	Luginina A.P. _____	117
Aranghel D. _____	77	Moscalu F. _____	118
Badita C.R. _____	77	Nabiev A.A. _____	120
Bairamukov V.Y. _____	79	Oprica L. _____	121
Balasoiu M. _____	81, 83, 85, 87	Putz A.-M. _____	122
Balasoiu-Gaina A.-M. _____	89	Rajewska A. _____	123
Bodnarchuk V. _____	92	Rečko K. _____	125
Bulat N.V. _____	93	Rogov A.D. _____	124
Byvshev I.M. _____	94	Rulev M.I. _____	127, 128
Dragolici A.C. _____	96	Ryzhykau Yu.L. _____	130
Erhan R.V. _____	98, 99	Sadilov V.V. _____	132
Gapchenko A. _____	101	Seliverstova D.V. _____	133
Gapon I.V. _____	102	Shemet D.B. _____	135
Gazdaru D. _____	104	Sirotin A.P. _____	137
Gille W. _____	105	Sluchevsky A.Y. _____	138
Hangan T.L. _____	107	Smyslov R. _____	140
Hashimov R.F. _____	108	Soloviev A.G. _____	141
Ion I. _____	110	Solovjeva T.M. _____	142
Kazantsev A.S. _____	112	Stan C. _____	144
Kichanov S.E. _____	113	Suyasova M.V. _____	146
Kondela T. _____	115	Vlasov A.V. _____	148
Kopitsa G.P. _____	116		

Authors List

Aldea N. _____	90, 97	Bugaev L.A. _____	91, 133
Almásy L. _____	38, 120	Bugrov A. _____	138
Andries M. _____	119	Bulat N.V. _____	91
Angelov B. _____	138	Bulavin L.A. _____	69, 100
Anghel L. _____	74, 96	Bunoiu M. _____	79, 83
Aranghel D. _____	75	Burzo E. _____	16
Arzumanyan G.M. _____	28	Buzatu D. _____	142
Asgerov E.B. _____	118	Byvshev I.M. _____	92
Askarov E.B. _____	106	Cherezov V. _____	115
Astashkin R.O. _____	115	Chetverikov Yu. _____	138
Avakyan L.A. _____	91, 133	Chilom C. _____	102
Avdeev M.V. _____	29, 38, 69, 100	Ciccariello S. _____	103
Badita C.R. _____	75	Creanga D. _____	50, 119
Badiu D. _____	105	Cristescu C.P. _____	142
Bairamukov V.Y. _____	77	Culea E. _____	97
Balasoiu M. _____	50, 79, 81, 83, 85, 87, 94, 100, 102, 108, 119, 123, 142	Damay F. _____	123
Balasoiu-Gaina A.-M. _____	87	Désert S. _____	37
Balejcikova L. _____	38	Dinca-Balan V. _____	45, 85
Balgavy P. _____	113	Dragolici A.C. _____	94
Baranchikov A.E. _____	114	Dragolici F. _____	94
Belenov S.B. _____	133	Dressel M. _____	58
Belenov S.V. _____	91	Ergasheva M.M. _____	115
Belushkin A.V. _____	60	Erhan R.V. _____	74, 90, 96, 97, 122, 130
Belyanchikov M.A. _____	58	Ezdakova K. _____	138
Beskrovnii A.I. _____	106	Feldman T.B. _____	60
Bica I. _____	79, 83	Filatov M.V. _____	55
Biernacka M. _____	123	Frielinghaus H. _____	37
Birsan V. _____	79	Gagkaeva Z.V. _____	58
Bodale I. _____	119	Gallova J. _____	113
Bodnarchuk V.I. _____	90, 130	Gapchenko A. _____	99
Bogorodskiy A.O. _____	115	Gapon I.V. _____	100
Borshchevskiy V.I. _____	99, 115, 128, 146	Gazdaru D. _____	102
Búcsi A. _____	44	Gille W. _____	32, 103
		Golubev E.K. _____	21

Authors List

Gordeliy V.I. _ 60, 99, 110, 125, 126, 128, 131, 146	Khokhlov A.R. _____ 63
Gorshkova Yu.E. _____ 138	Khripunov A. _____ 138
Gorshunov B.P. _____ 58	Kichanov S.E. _____ 81, 111
Grebenko A.K. _____ 58	Kirilov A.S. _____ 51, 135
Grigoras M. _____ 50	Klekotka U. _____ 123
Grinenko V. _____ 58	Koltsov M.A. _____ 67
Gubanova N.N. _____ 114	Kondela T. _____ 44, 113
Gurin V.S. _____ 111	Konev A. _____ 36
Gusach A.Yu. _____ 115	Kopcansky P. _____ 38, 100
Guterman V.E. _____ 133	Kopitsa G.P. _____ 114, 138
Hangan T.L. _____ 105	Kovalev Yu.S. _____ 51, 99, 108, 110, 122, 128, 139
Hanslik R. _____ 37	Kozhevnikov S.V. _____ 79
Haramus V.M. _____ 38, 138	Kozlenko D.P. _____ 111
Hashimov R.F. _____ 106	Kučerka N. _____ 40, 113, 126
Haus T. _____ 113	Kuklin A.I. _____ 51, 52, 60, 63, 90, 92, 99,
Hubčík L. _____ 44	_____ 108, 110, 118, 122, 125, 126, 128,
Iacomi F. _____ 34	_____ 131, 135, 136, 139, 140, 144, 146
Ianăși C. _____ 120	Kulvelis Yu.V. _____ 52, 144
Ilatovskiy A.V. _____ 36	Kurkin T.S. _____ 21
Ioffe A. _____ 130	Kvyatkovsky A.L. _____ 56
Ion I. _____ 108	Larichev Yu.V. _____ 54
Ionascu L. _____ 94	Lebedev D.V. _____ 36, 55, 67
Isaev-Ivanov V.V. _____ 36, 55, 67	Lebedev O.V. _____ 21
Islamov A.Kh. _____ 111, 121	Lebedev V.T. _____ 41, 52, 77, 83, 144
Ivanchev S.S. _____ 52	Len A. _____ 120
Ivankov O.I. _____ 44, 51, 58, 60, 87, 92, 94,	Leostean C. _____ 90, 97
_____ 110, 111, 113, 122, 125, 126, 128,	Letarova M.A. _____ 58
_____ 131, 135, 138, 139, 140, 142, 146	Lucaci M. _____ 108
Ivanov V.K. _____ 114	Luginina A.P. _____ 115
Jabarov S.H. _____ 106	Lungu M. _____ 108
Jaksch S. _____ 37	Lupu N. _____ 50, 87
Jestin J. _____ 37	Maharramov A.M. _____ 118
Jouve H.M. _____ 22	Mandes A. _____ 45, 85
Karimova E.M. _____ 106	Manoshin S.A. _____ 130
Katsaras J. _____ 18	Mantea E. _____ 108
Kazantsev A.S. _____ 110	Marinescu V. _____ 108

Authors List

Matejicek P. _____	71	Putz A.-M. _____	120
Michels A. _____	19	Rachkovskaya G.E. _____	111
Micu M. _____	94	Rada M. _____	90, 97
Mishin A.V. _____	115, 146	Rada S. _____	90, 97
Molcan M. _____	38	Rajewska A. _____	121
Molchanov V.S. _____	56	Rečko K. _____	123
Motovilov K.A. _____	58	Rogachev A.V. _____	51, 63, 83, 110, 122, 128, 139, 140
Murugova T.N. _____	44, 58, 60, 92, 128, 131	Rogov A.D. _____	122
Nabiev A.A. _____	118	Rulev M.I. _____	125, 126, 136
Navolan D. _____	105	Runov V.V. _____	43
Nazarov I. _____	36	Rychkov G.N. _____	36
Neov D. _____	106	Ryzhykau Yu.L. _____	99, 110, 125, 126, 128, 146
Nikitenko Yu.V. _____	79, 108	Sacarescu L. _____	50
Nikolaev M.Yu. _____	128	Sadilov V.V. _____	130
Onufriev A.V. _____	36	Safarik I. _____	38
Oprica L. _____	119	Satula D. _____	123
Ostrovsky M.A. _____	60	Savenko B.N. _____	111
Ozerin A.N. _____	21	Savii C. _____	120
Pana O. _____	90	Savinov M. _____	58
Pantina R.A. _____	55	Sedov V.P. _____	144
Patroi D. _____	108	Seliverstova D.V. _____	131
Petrenko V.I. _____	38, 100	Shemet D.B. _____	133
Petukhova T.B. _____	51, 135	Shibaev A.V. _____	63
Philippova O.E. _____	56, 63	Shiryaev A.A. _____	65
Pipich V. _____	138	Shvetsov A.V. _____	67
Pleštil J. _____	120	Shvetsov A.V. _____	36
Popescu A. _____	102	Sidoruk K.V. _____	58
Popov V.I. _____	92	Siposova K. _____	38
Pospiskova K. _____	38	Sirotn A.P. _____	51, 135
Pré P. _____	65	Sluchevsky A.Y. _____	136
Pribora V. _____	61	Smyslov R. _____	138
Primachenko O.N. _____	52	Socol C. _____	102
Prodan G. _____	45	Soloviev A.G. _____	51, 139, 140
Pronin A.A. _____	58	Soloviov D.V. _____	51, 85, 87, 110, 122, 126, 128, 135, 136, 139, 140, 146
Pryadchenko V.V. _____	91, 133	Solovjeva T.M. _____	139, 140
Puscasu E. _____	50		

Authors List

Soltwedel O. _____	100	Vangeli I.M. _____	92
Strabionyan V.V. _____	91, 133	Vartanyan N.A. _____	115
Stan C. _____	142	Vekas L. _____	100
Strbak O. _____	38	Vladareanu S. _____	105
Stuhrmann H.B. _____	22	Vladoiu R. _____	45, 85
Suciu R.-C. _____	90, 97	Vlasov A.V. _____	99, 110, 125, 126, 128, 146
Suyasova M.V. _____	144	Volkov V.V. _____	47, 65
Szekely N. _____	138	Voloshchuk A.M. _____	65
Szhogina A.A. _____	144	Vorobiev A.A. _____	100
Szymański K. _____	123	Waliszewski J. _____	123
Teixeira J. _____	24, 44	Yaguzhinsky L.S. _____	92
Teplova V.V. _____	92	Yakovleva M.A. _____	60
Thakiris V. _____	108	Zabelskii D.V. _____	125, 126
Tikhonov V.I. _____	77	Zaccai N.R. _____	25
Timko M. _____	38	Zagrai M. _____	97
Tkachenko A. _____	138	Zavialova A. _____	138
Toan D.N. _____	106	Zavisova V. _____	100
Tomchuk O.V. _____	69	Zhigunov A.N. _____	71
Torgashev V.I. _____	58	Zhukova E.S. _____	58
Uhríková D. _____	44	Zimmer O. _____	22
Utrobin P.K. _____	146	Zinoviev E.V. _____	99, 110, 125, 126, 128, 146

Small-angle X-ray pinhole camera system Rigaku: parameters and first results

Yu.S. Kovalev^{1,2}, D.V. Soloviov^{1,3}, O.I. Ivankov^{1,3}, A.V. Rogachev^{1,2},
A.V. Vlasov², Yu.L. Ryzhikau², E.V. Zinovev², P.K. Utrobin², V.I. Borshevskiy²,
V.I. Gordeliy^{2,4,5}, A.I. Kuklin^{1,2}

¹ Joint Institute for Nuclear Research, Dubna, Russia

² Moscow Institute of Physics and Technology, Dolgoprudny, Russia

³ Institute for Safety Problems of Nuclear Power Plants, NAS Ukraine, Kiev, Ukraine

⁴ Institute of Structural Biology J.P.Ebel, Grenoble, France

⁵ Institute of Complex Systems (ICS), ICS-5: Molecular Biophysics, Research Centre Juelich, 52425, Juelich, Germany

In this work we present main parameters and some results of measurements on small-angle X-ray installation Rigaku, MIPT, Dolgoprudny, Russia, with rotating anode source. The flux on the sample is 10^7 ph/s/mm², the beam diameter is 0.4-0.8 mm. X-ray scattering is detected by Gabriel-type detector with option of using image-plate detector simultaneously mostly for WAXS measurements. We made detailed description of instrument parameters and described its possibilities in wide-angle and small-angle range, the possibilities for samples environment (temperature holders, extension, grazing, etc.). We show raw (2D) and treated (1D) experimental data. Also we show opportunities for range extension in wide angles. A protocol for instrument calibration is detail described. The first results with lipidic membranes and proteins are shown [1-4]. The results are compared with experimental SANS data obtained on YuMO spectrometer, IBR-2, JINR, Dubna, Russia[5].

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**The structure of deterministic mass, surface and multi-phase fractals
from small-angle scattering data**

A.Yu. Cherny

Joint Institute for Nuclear Research, Dubna, Russia

We present general results on small-angle scattering (SAS) from deterministic (i.e., exactly self-similar) mass, surface and multi-phase fractals. We suggest a method of obtaining additional information from SAS data of deterministic mass fractals, such as the fractal iteration number, the scaling factor, and the number of structural units composing the mass and surface fractal. For a multi-phase system, we show that the qualitative question can be answered from SAS data whether one fractal 'absorbs' another one or they are both immersed in a surrounding homogeneous medium. Surface fractals are shown to be constructed as sums of mass fractals. It is shown that under certain conditions, SAS from a surface fractal can be explained in terms of power-law distribution of sizes of objects composing the fractal (internal polydispersity).

Oligomerization of the ionic self-complementary peptide study

V.V. Yegorov^{1,2}, D.V. Lebedev², Y.A. Yagudina¹, A.I. Kuklin^{3,4}

¹DMRB PNPI NRC KI, Gatchina, Russia

²Influenza Institute MH of Russia, Saint-Petersburg, Russia

³Joint Institute for Nuclear Research, Dubna, Russia

⁴Moscow Institute of Physics and Technology (State University),

vlacgur@omrb.pnpi.spb.ru

Conformational diseases such as amyloidosis, are one of the main causes of the loss of the capacity for self-care in the elderly. Amyloid fibril formation which underlies the pathogenesis of many conformational diseases have abnormal resistance to chemical and physical influences. From molecular modeling of the interaction of various proteins with a number of model molecules - structural nucleotide analogs, we found that, within the model used, these substances have a tendency to interact to beta-structured regions in proteins. Beta-strands are the main structural motif responsible for the formation of amyloid fibrils.

We studied the effect of nucleotides, a number of analogues of nucleotides and oligonucleotides at various stages of fibril formation of a peptide GDIRIDIRIDIRG (Egorov et al., 2008). The peptide comprises an ionic self-complementary motif (SCM), also described in the study of small heat shock proteins (D'Auria et al., 2009). These proteins provide SCM interaction between the subunits. For the assembly of functional chaperonins, which are oligomeric complexes must interact oriented antiparallel SCM monomers. It is shown that SCM is also involved in the interactions that determine the assembly of crystallin oligomeric complexes - the structure of the proteins found in various organs, including the eye tissues.

The model peptide GDIRIDIRIDIRG was studied by us previously. It was found that it has all properties that characterize amyloidogenic peptides and, at the same time, is simple for computer modelling and studying of its spatial structure and oligomerization using biochemical and biophysical methods such as SANS. The number of nucleotide analogs was tested as anti-amyloidogenic agents. It was shown that one of nucleotide analog is capable to react with basic side-chain groups of amino acid residues and, in some cases, capable to dissociation of amyloid-like fibrils.

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Magnetization distribution in non-collinear systems. The method

J. Waliszewski^{1,2}

¹ University of Białystok, Physics Faculty, Białystok, Poland

² JINR, Dubna, Russia

j.waliszewski@uwb.edu.pl

The magnetization, especially of the 3d electron systems, is built by the outer electrons, thus it can give precise insight into the distribution of the outer electrons in the unit cell in the crystal. It can be relatively easy found for the collinear magnetic systems. Nevertheless, the competitions between FM and AFM interactions, geometric frustration of AFM interactions or anisotropy caused by the preferred direction of magnetization are the sources of the non-collinear arrangement of the magnetic moments. The noncollinearity creates the significant troubles in the reconstruction of magnetization distribution in the unit cell. Complex magnetic systems are often studied by means of the polarized neutron diffraction with strong external magnetic field. In this technique the only one parameter – the flipping ratio R – is measured, and thus the determination of the vectorial map of the internal magnetization distribution is not easy.

Here I propose relatively simple method of the reconstruction of magnetization density distribution in non-collinear magnetic system. The only information desired are the unpolarized neutron diffraction data, collected without an external magnetic field. It can be shown that any non-collinear magnetic system can be reduced to a number of collinear magnetic systems, each of them associated with a given component of magnetic moments: any magnetic structure factor can be expressed as the combination of the “partial” magnetic structure factors each of them dependent on the different component of individual magnetic moment of the atoms in the system.. Then, for each of these “collinear” systems, the distribution of the proper component of magnetization can be easily reconstructed by the Maximum Entropy Method. The results of the method applied for hypothetical orthogonal and non-orthogonal crystallographic systems with different arrangements of magnetic moments in the unit cell are discussed. Then the method is applied for some real experimental data collected on the systems with the different with collinear and non collinear arrangement of magnetic moments. As an example the reconstruction of magnetization distribution as found for the non-collinear and incommensurate ScFe_4Al_8 [1] compound is presented.

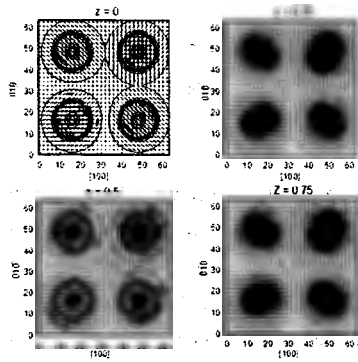


Fig. The magnetization density distribution in XY planes of ScFe_4Al_8 for different z coordinates. The every second point in each direction was shown for better readability. The length of the magnetisation vectors are given in a logarithmic scale. The number of 10 contours are drawn in linear scale in the regions from $0.0 \mu_B/\text{\AA}^3$ to $2.0 \cdot 10^{-3} \mu_B/\text{\AA}^3$ for $z = 0.0$, from $0.0 \mu_B/\text{\AA}^3$ to $5.0 \cdot 10^{-3} \mu_B/\text{\AA}^3$ for $z = 0.5$ and from $0.0 \mu_B/\text{\AA}^3$ to $1.45 \mu_B/\text{\AA}^3$ for $z = 0.25$ and $z = 0.75$.

[1] J.Waliszewski, K.Recko, Journal of Optoelectronics and Advanced Materials 17, No. 7-8 2015, p. 958

FLNP JINR User Program

D.M. Chudoba, Yu.E. Gorshkova, I. Zinikovskaia

Joint Institute for Nuclear Research, Dubna, Russia

Scientific_Secretary@nf.jinr.ru

Since 2012, the IBR high flux pulsed reactor (Dubna, Russia) [1] renewed regular operation at 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 Program[2]. Calls for proposals are issued twice a year. The proposals are peer-reviewed and rated and beam time for experiments is allocated on the basis of the reviews by Expert Committees. At present, 200 experiments per year are performed by scientists from more than 20 countries at IBR-2 instruments in the framework of the User Program.

[1] <http://flnp.jinr.ru/34/> - IBR-2 Pulsed Reactor

[2] <http://ibr-2.jinr.ru/> - IBR-2 User Club

502



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