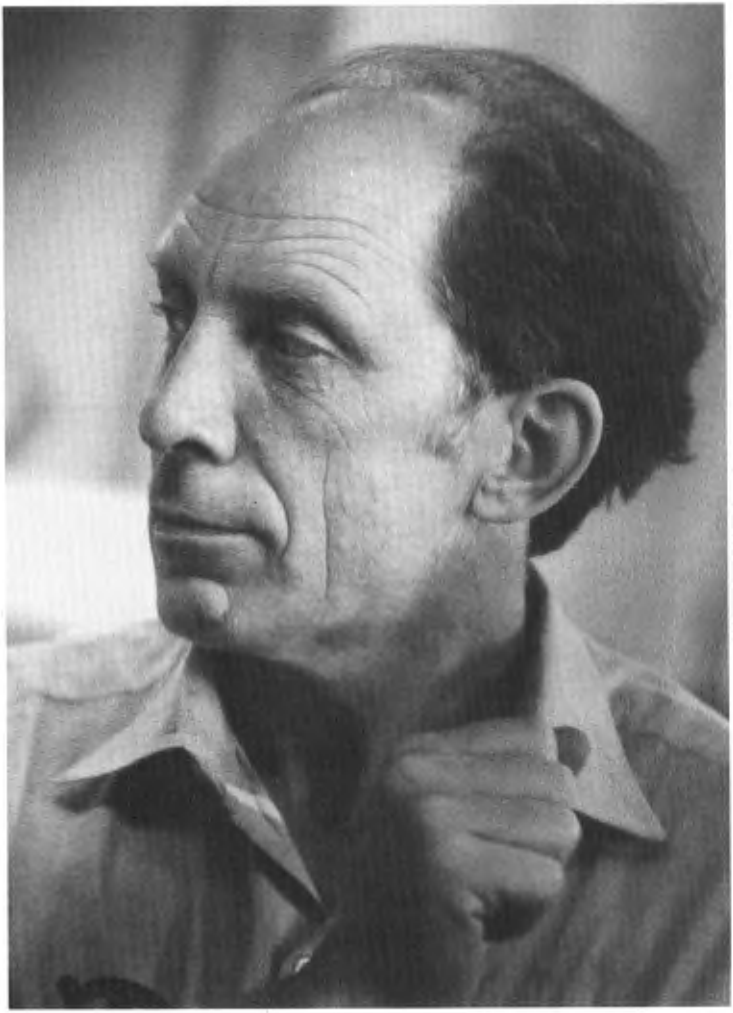
INTERNATIONAL SMALL-ANGLE SCATTERING WORKSHOP DEVOTED TO THE 70TH ANNIVERSARY OF YU. M. OSTANEVICH'S BIRTH

Programme and Abstracts of the Workshop



JOINT INSTITUTE FOR NUCLEAR RESEARCH
FRANK LABORATORY OF NEUTRON PHYSICS

INTERNATIONAL SMALL-ANGLE SCATTERING WORKSHOP DEVOTED TO THE 70TH ANNIVERSARY OF YU. M. OSTANEVICH'S BIRTH

Dubna, October 5–8, 2006

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Dubna • 2007

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УДК [538.9+539.125.5](092)
ББК 22.371.21я434
I 69

Sponsors and Financial Support

Frank Laboratory of Neutron Physics
Joint Institute for Nuclear Research
Grants of Plenipotentiaries of JINR Member States:
Czechia, Slovakia, Poland

The contributions are reproduced directly from the originals presented by the Organizing Committee.

International Small-Angle Scattering Workshop devoted to the 70th anniversary of
I 69 Yu. M. Ostanevich's birth: Programme and Abstracts (Dubna, October 5–8, 2006). — Dubna: JINR, 2007. — 60 p.
ISBN 5-9530-0149-5

Международное совещание по малоугловому рассеянию, посвященное 70-летию со дня рождения Ю. М. Останевича: Программа и тезисы докладов (Дубна, 5–8 октября 2006 г.). — Дубна: ОИЯИ, 2007. — 60 с.
ISBN 5-9530-0149-5

ISBN 5-9530-0149-5

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SAS Workshop Program

October 4, Wednesday

18.00 – 20.00 Registration

October 5, Thursday

International Conference Hall

9.00 – 10.20 Registration
10.20 – 10.50 The opening ceremony

Chairman: **G. Pepy** (Leon Brillouin Laboratory, Saclay, France)

10.50 – 11.40 Lecture: **A.M. Balagurov** (Frank Laboratory of Neutron Physics, JINR)
"A review of Yu.M. Ostanevich scientific activity"

11.40 – 12.10 Coffee break

12.10 – 13.00 Lecture: **J. Plestil** (Institute of Macromolecular Chemistry, Prague, Czech Republic)
"SANS Study of Associative Behaviour of Mixtures of Poly(ethylenoxide)/Poly(propylene oxide) Copolymers of Various Architecture"

13.00 – 13.50 Lecture: **A.R. Khokhlov** (Moscow State University, Russia)
"Small-angle neutron scattering study of responsive nanostructures in smart polymer systems"

13.50 – 15.00 Lunch

Chairman: **A. R. Khokhlov** (Moscow State University, Russia)

15.00 – 15.50 Lecture: **A. N. Ozerin** (Institute of Synthetic Polymer Materials RAS, Moscow, Russia)
"Complementary SAXS and SANS Studies of Dendrimers"

15.50 – 16.40 Lecture: **J. S. Pedersen** (University of Aarhus, Denmark)
"Structure and interactions of PEO-containing block copolymers micelles by small-angle scattering"

16.40 – 17.10 Coffee break

17.10 – 19.00 Excursion to the YuMO instrument at IBR-2 reactor

20.00 - Welcome party (in the **"Dubna" hotel**)

October 6, Friday

International Conference Hall

Chairman: **R. K. Heenan** (ISIS, Rutherford Appleton Laboratory, UK)

10.00 - 10.50 Lecture: **J. Teixeira** (Leon Brillouin Laboratory, Saclay, France)
"Demixtion of liquids in a porous material probed by SANS"

10.50 – 11.40 Lecture: **G. Pepy** (Leon Brillouin Laboratory, Saclay, France)
"Nanochannels in track etched membranes observed by SAS"

11.40 – 12.10 Coffee break

Chairman: **J. Teixeira** (Leon Brillouin Laboratory, Saclay, France)

12.10 – 13.00 Lecture: **R. K. Heenan** (ISIS, Rutherford Appleton Laboratory, UK)
"SANS data fitting"

13.00 – 13.50 Lecture: **G. Pepy** (Leon Brillouin Laboratory, Saclay, France)
"The PXY program for 2 (or 3) dimensions data treatment"

13.50 – 15.00 Lunch

15.00 – 16.10 Poster session/Discussions: Presentation of the YuMO activity

16.10 – 16.30 Coffee break

16.30 – 18.00 A tour around Dubna

19.00 - 21.00 **Remembering Yu.M. Ostanevich** (A.I. Kuklin, J. Plestil and all who knew Yurij Ostanevich)

Green room, International Conference Hall

October 7, Saturday

International Conference Hall

Chairman: **P. Balgavy** (Comenius University, Bratislava, Slovakia)

10.00 - 10.50 Lecture: **G. Zaccai** (Institut Laue-Langevin, Grenoble)
"Neutron scattering illuminates the dynamic structures of biological macromolecular complexes"

10.50 – 11.40 Lecture: **V.V. Chupin** (Shemyakin & Ovchinnikov Institute of

Bioorganic Chemistry RAS, Moscow)
"Lipid-coated nanocapsules (cisplatin nanocapsules)"

11.40 – 12.10 Coffee break

Chairman: **G. Zaccai** (Institut Laue-Langevin, Grenoble)

12.10- 13.00 Lecture: **D.V.Lebedev and V.V.Isaev-Ivanov** (PINPh, St. Petersburg, Russia)
"Chromatin organization in native interphase cell nuclei by SANS"

13.00-13.50 Lecture: **P. Balgavy** (Comenius University, Bratislava, Slovakia)
"SANS study of bilayer thickness and lipid surface area in unilamellar phosphatidylcholine vesicles"

13.50 – 15.00 Lunch

Chairman: **A. N. Ozerin** (Institute of Synthetic Polymer Materials RAS, Moscow, Russia)

15.00 – 15.25 Lecture: **A. Sokolova** (Institute of Crystallography, RAS, Moscow, Russia)
"On-line system DaRa for rapid protein characterization based on X-ray small-angle scattering"
15.25 – 15.50 Lecture: **A. Kuklin** (Frank Laboratory of Neutron Physics, JINR, Dubna)
"Development of SANS at IBR-2"

15.50 – 16.20 Coffee break

16.20 – 17.10 Lecture: **R. K. Heenan** (ISIS, Rutherford Appleton Laboratory, UK)
"Plans for Instrumentation at ISIS"

17.10 -18.00 The closing ceremony

October 8, Sunday

Conference Hall of Laboratory of Neutron Physics. Building 42.

Round table "Development of SANS"

Chairman: **J.S. Pedersen** (University of Aarhus, Denmark)

9.00 - 9.25 **G. Pepy** (Leon Brillouin Laboratory, Saclay, France)

"New collimation systems - projects and results"

9.25 – 9.50 **G. Zaccai** (Institute of Laue-Langevin, Grenoble)
"New SANS instrumentation at ILL"

Chairman: **V.I. Gordeliy**

09.50 – 10.15 **J.S. Pedersen** (University of Aarhus, Denmark)
"SANS data fitting"

10.15 – 10.55 **Discussions**

10.55 – 11.00 Closing remarks

11.00 – 11.20 Coffee break

11.20 - 22.30 Excursions

Preface

Time-of-flight small-angle neutron scattering at IBR-2

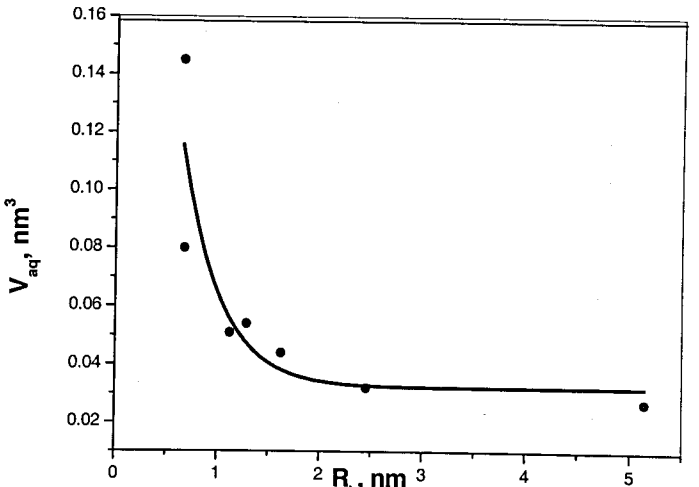
A. Kuklin, A. Islamov, T. Murugova, V. Gordeliy

The issue contains abstracts of the lectures and posters presented at International Small-Angle Scattering Workshop devoted to the seventieth anniversary of an outstanding physicist - professor Yuriy Mechislavovich Ostanevich (1936-1992), who was the founder of SANS at Frank Laboratory of Neutron Physics. It is a great pleasure for us to give a brief introduction to Prof. Yu.M. Ostanevich scientific activity related to small-angle neutron scattering. Three of the authors of this introduction (AK, AI and VG) knew and worked with him. One of us (TM) came to the Laboratory when he left us, but we all benefit from the beautiful science, the YuMO instrument and the scientific spirit, which Yu.M. Ostanevich had created for us and our colleagues.

Prof. Yu.M. Ostanevich had broad knowledge and deep understanding of physics. This allowed him to enter quickly a new scientific field and work there efficiently. He started his research with the studies of the Mössbauer effect in condensed matter in the sixties. One of his activities was investigations of the effect of gravity on self-diffusion at critical point of water and neutron resonances. Since 1974 he concentrated on creating a first time-of-flight small-angle spectrometers at IBR-30 and IBR-2 pulsed reactors. We and our colleagues who are working at the YuMO SANS instrument at IBR-2 are aware of the outstanding quality and longlivity of Yu. M. Ostanevich's scientific and technical ideas lying in the basis of the instrument. Already the first SANS studies done by Yu. Ostanevich and his colleagues are impressive and show how wide his scientific interests were. The publications on the studies of biological macromolecules [1-3], polymers [4-6], lipid membranes [7,8], small molecules [9,10] and micelles [11-13] nicely illustrate this.

Let us give an example of an important work by Yu. M. Ostanevich and his colleagues. To our opinion, the series of articles, which were written quite a long time ago by N.I. Gorskiy and Yu.M.Ostanevich are still very interesting today [11-13]. N. Gorskiy and Yu. Ostanevich turned to the remarkable ability of the surfactants to form invert micelles in hydrophobic solvents (e.g. in C_6H_6 and CCl_4). The surfactant sodium 1,4-bis-(2-ethylhexyl)-sulphosuccinate (AOT) forms invert spherical micelles with the central water kernel of radius $R_h=A+K(C_w/C_s)$, where C_w and C_s are concentrations of water and surfactant correspondingly and A and K are the constants. Therefore this system provides a unique opportunity to study

water droplets with very small radius in the range of ~10–100Å by changing the water/surfactant ratio in the system. The Fig.1 shows the dependence of the experientially



Dependence the volume per single water molecule on the radius of the water kernel (solid circles - experimental results)

obtained value of the volume per single water molecule V_{aq} on the radius of the kernel R_h. It is apparent that in the case of a small radius of the kernel the volume greatly exceeds the volume of water molecule in bulk (30 Å^3). However, the volume per single water molecule approaches 30 Å^3 at R_h >20 Å.

Another example of fruitful activity of Yu. M. Ostanevich is the review written together with I.N. Serdyuk [14]. It was written before the SANS spectrometer at IBR-2 was commissioned and came just a right time and was appreciated by the biological scientific community interested in applications of SANS to their biological objects. In this review the authors examined theoretical and practical problems of application of small-angle scattering in biology.

Yu.M. Ostanevich actively applied SANS to studying small molecules [15,16]. Such experiments are not trivial because the scattering from small objects is weak and the experiments require excellent experimental skills, which Yu. M. Ostanevich certainly possessed.

Investigations of polymers at the MURN spectrometer were started by J. Plestil and Yu. M. Ostanevich with polyelectrolytes. Hydration and the local structure of polyions, binding of counterions to polymers were the first problems addressed in [17,18]. The interpolyion correlations and the size of polyions were obtained in [19,20]. The Nylon-6 in swollen state [21] and thermosensitive gels [22,23] were studied by SANS at the MURN instrument. A more detailed account about the investigations of polymers as well as block copolymer micelles (corona micelles, three-layer micelles and nanoparticles) can be found in the papers and reviews by J. Plestil, who was one of the closest co-workes of Yu.M.Ostanevich [24-26].

At present, the investigation of polymers at the YuMO spectrometer at IBR-2 is one of the most active fields. It is also worth to mention here important studies done by the known polymer schools of Prof. A. R. Khokhlov and Prof. A.N. Ozerin. Among these works are investigations of self-assembly polyelectrolyte rods in polymer gel and in solution [27] and a new type of polymers – dendrimers [28-32], the charge-induced microphase separation in polyelectrolyte fenomena [33-35], poly(ethylene oxide)/poly(propylene oxide) copolymers in aqueous solution [36].

Yu. M. Ostanevich devoted continuous attention to the development of time of-flight methodology and the instruments at IBR-30 and IBI-2 pulsed reactors. His first ideas and experimental results on time-of-flight SANS were published in 1977 [37]. The first experiments with proteins in solutions confirming the method as well as the basic characteristics of the spectrometer were briefly described in the publication. It is interesting to note that a new type of detector of thermal neutrons for the SANS instrument – circular multi-wires He^3 detector with a central hole were presented before this publication. Namely such a detector was the main part of data acquisition system of SANS instrument at IBR-2 during more than 20 years. Later this type of the detectors allowed us to propose and experimentally realize in 2000 a new approach to the collection of time-of-flight SANS data by using two detector system at the YuMO [38].

Yu.M. Ostanevich was an outstanding scientist and being deeply involved in nearly all the experiments done at the machine he understood well the users of the instrument. He was always trying to improve the instrument without shutting down the machine at the time when the reactor was in operation. The SANS group tried to preserve this good tradition doing modernization of the instrument, installation of a two detector system as well as a new type of two dimensional position sensitive detector at the YUMO [39]. We know now how much extra efforts Yu.M. Ostanevich had to apply to keep the instrument in operation continuously modernizing it.

Yu.M. Ostanevich launched one of the most efficient scientific schools at the Laboratory working for a very wide scientific society in Russia, JINR member countries and others. Let us very briefly mention just some of the present scientific activities at the YuMO:

***biophysics*:** research on model and biological lipid membranes, their structure, properties and interactions; interactions of membranes with biologically active molecules; structure of membranes and biomolecules under high pressure; membrane proteins: their structure, interactions with detergents, structural changes, behaviour of lipidic systems in couse of membrane protein crystallization [40-45];

physical chemistry of surfactants and colloids: investigations of behaviour of micellar solutions under normal conditions as well as under high pressure in a wide temperature range, in particular, kinetics of phase transitions of micellar solutions to crystals under high pressure [46-50];

***polymer physics*:** studies of structure, properties and self-assembly of modified polymer gels; structure of polymer gels with covalent and non-covalent bound hydrophobic chains to understand a regulation of responsive properties of the gels; association behavior of PEO/PPO star copolymer with hydrophobic terminal blocks in aqueous solution and micelle solutions of three-layer nanoparticles prepared by polymerization of methyl methacrylate in polystyrene-*block*-polymethacrylic acid and polymethyl methacrylate-*block*-polymethacrylic acid; structure of polycarbosilane dendrimers with different molecular architecture (shapes and sizes to be determined to clarify controversial literature data on properties of dendrimers) [27-36, 51];

nanoparticle and material science: investigations of structure of technical and biocompatible ferrofluids (effect of magnetic particle concentration and temperature variation on the structure of mono and double layer stabilization of ferrofluids); properties of FeCu alloys; structure of nanoparticles of C_{60} under different conditions as well as different kinds of artificial membranes and soils [52-65];

mathematical methods of data treatment: development of new methods of treatment of SANS data in case of weak statistics [66]; creation of a new program to treat SANS data obtained from PSD detector as well as software package for the YuMO spectrometer [67] and data treatment [68,69].

The IBR - has been recently shut down for reconstruction. This is the right time for a principal modernization of the YuMO and one of the challenges is the adaptation of the SANS instrument to the cold neutron source at IBR-2. The participants of the workshop spent some extra time suggesting interesting ideas about the principal modernization of the YuMO. They believe that one of the most productive methods and instruments at IBR-2, the YuMO

launched by Yu.M. Ostanevich and further developed by his team will get sufficient support to be ready for future successful work when IBR-2 will be in operation again.

Acknowledgements

The workshop attracted leading scientists of the world who are exploiting and developing SANS and neutron diffraction and we are very grateful to A. Balagurov, A. Belushkin, P. Balgavy, V. Chupin, G. Eckold, R. Heenan, V. Isaev-Ivanov, A. Khokhlov, D. Lebedev, J. Pederson, G. Pepy, J. Plestil, A. Sokolova, A. Ozerin , J.Teixera, G. Zaccai for high level of scientific and human atmosphere which they brought with them to us. We would very much like to thank T. Ostanevich as well as the colleagues and friends of Yu.M. Ostanevich for attending a special Workshop's event devoted to the memory of Yu.M. Ostanevich. We were happy to feel the generous support of the members of the Organizing Committee: N. Malisheva, V. Novikova, A. Sustina, A. Balagurov, S. Yarovikov, A. Rogachev, Yu. Kovalev, S.Ph.Yarovikov, A. Ivankov,and V. Simkin.

We also express our gratitude to the sponsors of the Workshop: the Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research and the JINR member countries Czech Republic, Slovakia and Poland.

And last, but not least we would like to thank V. Aksenov, A. Belushkin and S. Kozenkov for important support of the Workshop in Dubna.

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Lectures

SANS STUDY OF BILAYER THICKNESS AND LIPID SURFACE AREA IN UNILAMELLAR PHOSPHATIDYLCHOLINE VESICLES

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It is well known that functional properties of transmembrane proteins critically depend on physical properties of the lipid bilayer. In particular, the phosphohydrolysing activity of sarcoplasmic reticulum (Ca-Mg)ATPase (SERCA) reconstituted into fluid bilayers from synthetic diacylphosphatidylcholines with monounsaturated acyl chains (diCn:1PC, n is the number of acyl carbons) displays a maximum for diC18:1PC and decreases progresivelly for shorter and longer acyl chain lengths [1,2]. This effect is explained by the „hydrophobic mismatch" between the bilayer and the hydrophobic part of the protein [2]. The SERCA activity is also modulated by the presence of various bilayer admixtures such as decane (C10), cholesterol (CHOL) or amphiphilic *N*-dodecyl-*N*,*N*-dimethylamine-*N*-oxide (C12NO) [1-3]. We have used SANS on unilamellar diCn:1PC vesicles to find which bilayer parameters could be responsible for the modulation of SERCA activity by the diCn:1PC acyl chain length and by the bilayer admixtures of C12NO, C10 and CHOL. From SANS spectra, we have obtained the bilayer gyration radius R_g and the bilayer thickness parameter $d_g = 12^{0.5}R_g$. Using a model of the bilayer scattering length density profile inspired by molecular dynamics simulations [4], the steric bilayer thickness d_S, the surface area A_L per lipid at the bilayer – aqueous phase interface and the number of water molecules n_W per lipid located in the bilayer polar region have been obtained from SANS spectra of diCn:1PC vesicles. The results indicate, that the SERCA activity is modulated by a delicate interplay of several physical factors, and not only by the „hydrophobic mismatch".

Acknowledgements: The experiments were supported by the EC through NMI3, Contract n°: RII3-CT-2003-505925; by the JINR project 07-4-1031-99/2008, by the VEGA grant 1/3029/06, and by the APVV grant 51-027 404.

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SMALL ANGLE SCATTERING FACILITIES AT THE FRM-II

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The new neutron source FRM-II in Garching provides excellent conditions for all the different fields of neutron scattering. The first suite of instruments, both in the experimental hall around the reactor as well as in the neutron guide hall, is currently in routine operation and the first user experiments have successfully been performed. The decision to shut down the Juelich reactor and to transfer the most suitable instruments to FRM-II greatly improves the situation of small angle scattering. Two conventional SANS-instruments, KWS1 and KWS2, are currently being installed in the neutron guide hall along with the focusing mirror instrument KWS3. Moreover, the new facility SANS-1 is under construction which provides a sophisticated neutron guide system for polarized neutrons that is optimised to use most effectively the high flux provided by the cold source. In this contribution, a short overview about the current status of the SANS-activity at FRM-II will be given.

FITTING SANS DATA - SOME PRACTICAL ADVICE

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The interpretation and fitting of SANS data can often take far longer than preparing the samples or collecting the data. This talk will introduce the fitting techniques that are possible and will mention some of the software that is available to help in the task of getting the best out of hard won SANS data. Two of the most general programs are the stand alone FISH [1], and routines from NIST which run within a free demonstration version of the commercial IGOR data manipulation package [2]. Programs CRYSON, DAMMIN, SASHA etc. within the well known ATSAS package from EMBL [3] are mostly aimed at monodisperse biomolecules, though the MIXTURE program may be useful in other fields. Many other codes are available, particularly for more specialised cases.

[1] http://www.isis.rl.ac.uk/largescale/loq/loq.htm

[2] http://www.ncnr.nist.gov/programs/sans/data/data_anal.html

[3] http://www.embl-hamburg.de/ExternalInfo/Research/Sax/software.html

PLANS FOR SANS INSTRUMENTATION AT ISIS

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With considerable good fortune the ISIS facility is progressing with the building of a second spallation target optimised for the production of cold neutrons. This will take one pulse in five from the 50 Hz, 800 MeV ISIS proton synchrotron (being upgraded from 200 to 300 μA). A small target with a composite, coupled, grooved, cold moderator will give a large increase in flux compared to the existing target. This 10 Hz cold neutron source will enable world class SANS and Neutron Reflection beam lines to be operated. Three reflectometers (INTER, offSPEC, POLREF) and one SANS instrument (SANS2d) are amongst the day one beam lines. The SANS2d instrument will have two 1m square detectors in a 3.5m diameter vacuum tank, with sample-detector distances of between 2 m and 12m. Technical details and scientific goals of the SANS2d instrument will be described.

Further SANS instruments are proposed, though no funding is available at present. These include SPIRAL, a time-of-flight spin-echo SANS machine, which will use techniques already being developed in collaboration with the University of Delft for the offSPEC reflectometer. ZOOM is envisaged as a conventional SANS instrument with a large and flexible sample space that could also be used for development of focussing techniques with lenses or mirrors. Both these beam lines have the potential to reach much smaller Q than at present, thus opening up new areas of science to the advantages of neutron scattering.

CHROMATIN ORGANIZATION IN NATIVE INTERPHASE CELL NUCLEI BY SANS

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While substantial amount of knowledge has been accumulated about molecular mechanisms of genetic processes, little is know about the integration of these processes in the structure of the cell nucleus. To understand the functional organization of genome it is important to uncover the main principles of the cell nucleus architecture. This calls for an experimental approach that would allow to investigate the structure of the nucleus in its native state on broad range of scales.

Small angle neutron scattering yields information about the general principles of chromatin organization on the range of scales that cover the entire hierarchy of the chromosomal structures from nucleosomal to the nucleus as a whole. In addition, it allows to distinguish the contribution of the protein and nucleic component into the structure of nucleus.

Cell nuclei of higher organisms, such as nuclei of chicken erythrocytes and rat lymphocytes were subject of collaborative study by the laboratories of Cell Biology and Biophysics of Macromolecules DMRB PNPI. The results obtained so far show three levels of chromatin organization: the region of nanoscales (down to the size of the nucleosome, large Q), region of scales close to the size of the nucleus (very small Q) and the fractal region.

Interference maximum and undulations observed in the first region of SANS spectrum (Q ~ 0.02 - 0.05 $Å^{-1}$) are characteristic of the nucleosomal structure. The shape of the curve in this region and the position of the maximum depend on the mean distance between nucleosomes and the degree of compaction of the nucleosomes themselves. Compared to control nuclei, in cell nuclei subjected to ethidium bromide or RNase treatment, or to gamma radiation, these parameters related the nucleosomal structure are markedly different.

In the region of the scattering vector magnitudes between $3 \cdot 10^{-4}$ до $3 \cdot 10^{-2}$ $Å^{-1}$ (characteristic scales between 20 nm and 2 μm) SANS spectra of cell nuclei have two regions that linearize on a double-exponential scale. The power law dependency of the scattering intensity on the magnitude of the scattering vector, $I(Q) \sim Q^{-D}$, indicates the fractal structure of cell nuclei. Nucleic (DNA+RNA) components of chromatin, studied by contrast variation, have been shown to have two fractal regions, one from $2 \cdot 10^{-2}$ $Å^{-1}$ to $2 \cdot 10^{-3}$ $Å^{-1}$ (linear scales from 30 to 300 nm) with the dimension $D_m \sim 2.2$ (mass fractal), and the second surface fractal region from $2 \cdot 10^{-3}$ $Å^{-1}$ to $3 \cdot 10^{-4}$ $Å^{-1}$ (scales from 300 nm to 2 μm). The Flory exponent for the nucleic component on the scales from 30 nm to the crossover point (300 - 400 nm), estimated from SANS spectra, was very similar for the chromatin of chicken erythrocyte and rat lymphocyte nuclei, close to 0.45. Thus, the structure of the nucleic component of chromatin on the smaller scales resembles Gaussian chain, while on the larger scales it is seen as a surface fractal.

SMALL-ANGLE NEUTRON SCATTERING STUDY OF RESPONSIVE NANOSTRUCTURES IN SMART POLYMER SYSTEMS

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The paper is devoted to the study of the self-organization in amphiphilic polymer gels arising as a result of competition of two counteracting tendencies: hydrophobic aggregation and electrostatic repulsion.

The objects of the investigation are the gels based on copolymers of acrylic acid and n-alkylacrylate. Variation of the fraction of hydrophobic units and of the length of their n-alkyl substituent allows one to control the hydrophobic properties of the gel, while the change of the degree of ionization of acrylic acid units gives the possibility to regulate the electrostatic repulsion.

By SANS it was observed that the gel ionization induces the microphase separation with the formation of hydrophobic regions containing densely packed hydrophobic aggregates that alternate with hydrophilic regions highly swollen by water, where most of charged units and counter ions are located. It was shown [1] that increasing degree of ionization of the gel (triggered by pH) induces a tremendous decrease of the size of hydrophobic regions. Therefore, the gels of hydrophobically modified poly(acrylic acid) are able to self-organize with the formation of microdomain structures, the period of which can be varied significantly by slight changing of the pH value of the medium, which determines the degree of ionization of the gel.

The dimensions of the nanostructure of the gels with quenched and annealed charged groups were compared [2]. It was shown that the size of hydrophobic regions in the gels with annealed charged units is much bigger than in the gels with the same fraction of quenched charged units. This effect was attributed to much weaker electrostatic repulsion in the corona of the hydrophobic regions in the gels with annealed charged groups, because the charged units repelling each other are able to move farther apart.

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Acknowledgement. The financial support of RFBR (project 05-03-32865) and Grant of President of RF (MK-5173.2006.3) is acknowledged.

DEVELOPMENT OF SANS AT IBR-2

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The modernized YuMO is the most user requested instrument at the IBR-2. The users of the YuMO instrument from JINR member state and German institutes together with the members of the SAS group have justified the efficiency of their research work by outstanding record of scientific publications. The key element of modernized YuMO spectrometer is two detector system (TDS) [1,2]. The new setup of the instrument allows to collect simultaneously SANS data in a wide interval of scattering vectors. However, in 2010 the YuMO will face new challenges. During nearest years ILL, Grenoble is planning to install new additional SANS instruments, new neutron scattering centers in Garhing (FRG) and Oak Ridge National Laboratory (USA) will be equipped by high quality SANS instruments.

To ensure a proper place of the YuMO among world leading instruments of 2010 the YuMO should be modernized using 2 two-dimensional position sensitive detectors [3] in the way described below and will cover a wide range of Q: from 2×10^{-3} to 1 $Å^{-1}$, will have a unique resolution, Q_{max} and dynamic range of about 300. In addition, for the first time it will open a wide field of researches related to the studies of anisotropic objects.

The whole project can be executed in the following way: working out of the detector, electronics, hard- and software; manufacturing and assembling of the detector system including the parts necessary for its installation in the detector vacuum tube; the tests of the detector and its installation; modification of the front end of the detector vacuum tube to increase maximum available value of the scattering vector Q_{max}; adaptation of sample environment to studies anisotropic objects and the software for data treatment at the YuMO with 2D PSD system.

The sample environment should be adapted to the new set up of the instrument. Recently the equipment for creation of high magnetic field has been assembled. It will be installed and tested in the user mode at the YuMO. A number of scientific projects concerning SANS studies of anisotropic systems require orientation of the objects. This allows one to extract more information from experimental data. Reological study of polymer, surfactant, etc. systems is an efficient approach to investigate properties of these systems. All leading SANS instruments have corresponding equipment for the studies. It is planned to work out, manufacture and install the equipment at the YuMO. Taking into account high impact of SANS on investigation of condensed matter and high request for SANS by scientific community the SAS group has been suggested the installation of an additional and complementary to the YuMO SANS instrument at one of the most bright neutron beams of the IBR-2. Realization of projects would lead to creation of SANS spectrometer with world level of the parameters.

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COMPLEMENTARITY OF SANS AND SAXS STUDIES OF DENDRIMERS

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The structure determination of nano-sized objects is a hard task, especially for the case of dendritic (treelike, highly branched) structure of nanoparticles, where the interpretation of the experimental results is highly dependent on the *a priori* model selected to represent the spatial structure of nanoparticles.

This paper presents the results of the restoration of low resolution shape and internal structure of the dendritic nanoparticles of various chemical structure in solution (dispersion) from SANS and SAXS data made without *a priori* information on dendritic structure (*ab initio*).

In this study we have examined highly branched regular polymer structures (dendrimers). SANS and SAXS were used to determine precise numerical values on size, shape, partial volume and end group localization for the model set of polyallylcarbosilane dendrimers (generation number from 4 to 9) in diluted solutions.

The SANS experiments were done at the YuMO instrument equipped with a two-detector system at the IBR-2 reactor of FLNPh JINR (Dubna). The time-of-flight counting method was used to give the overall range of momentum transfer of $0.08 < s < 4$ nm^{-1}. The SAXS measurements were done using a KRM-1 camera (Bourevestnik, Inc.) with a slit collimation system, giving an overall range of momentum transfer of $0.07 < s < 4.26$ nm^{-1}. The SAS measurements were performed with the diluted (1÷2 wt.-%) solutions (dispersions) of the nanoparticles in the appropriate solvents at 25 °C.

The programs PRIMUS, GNOM, MASHA, SASHA and a bead modeling method implemented in the *ab initio* Monte Carlo-type simulated annealing program DAMMIN of the ATSAS 2.0 program complex [1] were used for the data treatment, structure evaluation and dendritic nanoparticles shape determination in this work.

The bead and envelope models reveal for the dendrimers anisometric shapes but also pronounced heterogeneity of the internal structure allowing for penetration of solvent molecules. The *ab initio* models agree astonishingly well [2] with the recent independent results of molecular dynamics simulations on dendrimers.

The results obtained gave a possibility to resolve many other contradictions in accounting for the results coming from the experimental methods applied to study structure and dynamics of dendrimers: IR, ESR, NMR, radiothermoluminescence, molecular modeling etc.

The authors are thankful to Prof. D.I. Svergun for helpful discussion. This work was funded by the Russian Foundation for Basic Research (grants ## 05-03-33120, 05-03-08124).

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STRUCTURE AND INTERACTION OF PEO-CONTAINING BLOCK COPOLYMER MICELLES BY SMALL-ANGLE SCATTERING

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Numerous studies of block copolymer micelles formed in selective solvent by scattering methods have been published in the literature. Many of the systems are contain PEO block as the soluble block in water. The PEO polymer forms hydrogen bonds with the water molecules and this is what renders it water soluble. Increasing the temperature reduces its solubility due to the gradual disordering of the hydrating water molecules and at 80-100°C [1], the theta temperature, water changes from being a good solvent to a becoming a poor solvent. It has been suggested [2] that some of the block copolymer systems have attractive intermicellar interactions and forms colloidal attractive glasses at high temperature and high concentrations. In order to investigate this further we have chosen a model system with the diblock copolymer Brij700 (C18 EO100) in water (D2O). The high asymmetry of the molecule and the high hydrophobicity of the C18 block suggest that spherical micelles can be present in a large temperature range. This was confirmed by SANS and SAXS measurements [3,4], which in addition gave information on intermicellar interactions. The data was analysed using expressions based on results from Monte Carlo simulations on models with a compact core and a corona of interacting, self-avoiding chains [5]. An effective hard-sphere structure factor was for describing the interactions effects and it did not reveal any signs of attractive interactions up to temperatures of 90 °C. The scattering results have further been supplemented by zero-shear viscometry and membrane osmometry [6], which confirms the conclusions from the scattering studies. The zero-shear viscometry has futher been used for deriving a more correct form for the intermicellar interaction potential, than the simple hard-sphere potential.

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Channels in track etched membranes observed by X-ray and neutron scattering

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Track membranes are thin polymer foils irradiated by heavy ions [1,2]. The defects created by the heavy ions are located along the ions trajectory: the track. It is possible to open channels by etching with a chemical agent. These channels are very uniform. Therefore these membranes can be readily used for filtration. They are also more and more used as templates for metallic wires replica prepared by soft chemistry. They might also be an interesting matrix to graft and study materials which cannot be crystallized (proteins) or to prepare nanocomposites.
Small Angle Scattering of X-rays (SAXS) and neutrons (SANS) give global information about the characteristics of the channel shape. As the nanochannels are strictly parallel, an excellent sample orientation is required to obtain interpretable spectra. Then oscillations of the Bessel function (radial part of the channel shape Fourier transform) are easily seen in the scattered intensity [3] (figure 1).
Recent developpements in a multipurpose XY data treatment software [4] allowed modelling the 2 dimensional SAS pictures, improving significantly the reliability of the interpretation.
SAXS measurements (on ID01 line in the ESRF) have been performed along SANS experiments on polyethyleneterephtalate (PET) and amorphous polycarbonate (aPC); the later exhibits channels with very small roughness. We present here a comparative study of one PET and 3 aPC which have been irradiated in GSI by the same heavy ion beam (Xe ions 11.1 MeV/u), each at 3 fluences ($3x10^8$, $5x10^8$,10^9 ions/cm^2) were used; each sample has been etched in 5N NaOH at 60°C, with or without UV sensitization, with 3 durations (3, 5, 8 min).The main results are:
- the amorphous polycarbonates always provide better channels than polyethylenterephtalate, however there are big differences between the polycarbonates, not only in the quality but also in the absolute value of the channel diameters,
- there is a systematic effect of the UV sensitization, which increases very significantly the quality
- depending of the channel diameter one may observe a negative effect of the larger fluences on the quality. Certainly one may expect that an increasing number of interacting channels destroys the uniformity of the channels. Meanwhile it seems that the interaction between channels takes place more often than the calculation tells.
- the quality of the smaller channels is worse than that of the biggest. It might be possible that a large halo around the original track makes the etching rougher and eases the connection between neighbouring channels.

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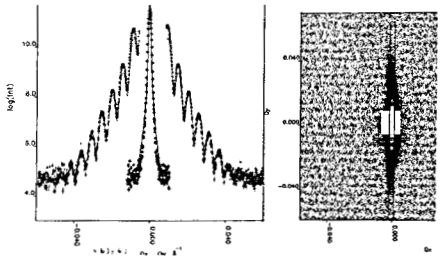

Fig 1. On the right, the SAXS by an aPC, 5.10^8 Xe/cm^2 irradiated, UV sensitized, 5 min etched. On the left a fit to the pixels in a vertical and a horizontal cut.

2D SAS : DATA TREATMENT; REMEDIES TO POOR INTENSITIES

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1 - 2D data treatment.

A new software performs data treatment of complex SAXS and SANS files.
Formats. This software can read many data formats (ESRF, ILL, LLB, Argonne, HMI, Jülich, BNC, Bruker...). It can display colour maps of one or several data files, up to 16 files simultaneously, with 25 colour palettes and several representations (straight, log, square root...).
Displays. A large variety of filters is available: rectangular horizontal or vertical or oblique cuts, or sector cuts, with display of the intensity versus x,y,ρ,θ accordingly. Also a rectangle pair (horizontal + vertical) is very useful in many cases (figure 1).
Models. While 1D model functions are available, this software is best with 2 dimensional modelling: classical gaussian, lorentzian and power functions with their combinations; also models for sphere, ellipsoid and cylinders, filled or hollow, with any orientation versus the incoming beam. These functions are centred on the beam or at any other position. It is possible to make linear combination of these functions or to modify them by specific form factors ("correlation hole", magnetic form factor). Symmetry rules may be applied to the functions. Simultaneous fits on several files are available. Most of the functions are provided with the option of applying size distribution laws. The effect of various apparatus resolution is included.
Fits. The current fitting procedure is a χ^2 least square process. In 2006 the MINUIT fitting package from CERN will be implemented. Several aids exist, for instance it is possible to map the difference between a data and a model files, the model as a measured data map, the χ^2 versus 2 parameters.
Displays. A very large number of ways to display the data maps, filter contents and models is available. All were designed to be friendly user to the experimentalist.
Code. This software is written in FORTRAN with the *pgplot* [1] graphic package.
References
[1] http://www.astro.caltech.edu/~tjp/pgplot/

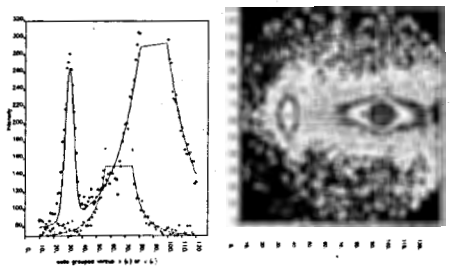

Fig 1 On the right data file for SANS by a liquid crystal polymer. It exhibits a central scattering due to the contrast between deuterated and protonated polymer chains and a Bragg peak characteristic of an overall smectic layers organization. For this example the 2 dimensions model included a centered anisotropic lorentzian for the forward scattering and a non centered gaussian-lorentzian function for the Bragg peak. A display limited to a pair of rectangular filters is shown on the left.

2 - Remedies to poor intensity

Pixels in complex or simply anisotropic pictures cannot be binned. Therefore the statistics of larger Q pixels is usually poor. The best remedy is to improve the intensity coming to the sample. This is usually achieved by keeping a large solid angle for the incoming beam, thanks to the input of a neutron guide in the collimator. It will be argued that a removable straight neutron guide would scarcely worsen the spatial resolution and the wavelength spectrum of YuMO, while increasing a lot the intensity, when necessary. With the exception of single crystals, large samples can accomodate multibeams converging at the detector position, further enhancing the intensity.. The first multibeam was long ago installed at the Argonne SAS. A very simple, "cross" configuration, with 4 sub-beams has been successfully built at the Budapest SAS. A Very Small Angle Spectrometer with multibeams is under development at the LLB.

SANS STUDY OF ASSOCIATIVE BEHAVIOUR OF MIXTURES OF ETHYLENE OXIDE/PROPYLENE OXIDE BLOCK COPOLYMERS OF VARIOUS ARCHITECTURE

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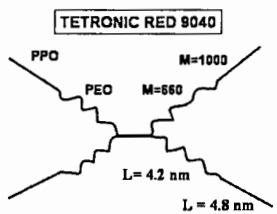
Structure of Tetronic RED 9040, a reverse-type (with hydrophobic terminal blocks) four-arm star polymer with ethylene oxide/propylene oxide (PEO/PPO) arms attached to the ethylenediamine core (See Scheme) was investigated in D_2O at concentrations between 0.2 and 50 g/dL in the temperature range from 15 to 75 °C.



At low temperatures and concentrations the copolymer was shown to be molecularly dispersed. This was indicated both by classical method of the molecular weight determination and the method not using the absolute scattering intensities and contrast factor [J. Pleštil, Makromol. Chem., Macromol. Symp., 15, 185 (1988)).

Upon increasing temperature (above ca. 40 °C) water becomes a bad solvent for PPO and the copolymer self-assembles to form an ordered structure.

The SANS curves exhibit a single scattering maximum with a characteristic (Bragg) distance of 8 nm independent of the copolymer concentration and only slightly dependent on temperature. This indicates that the maximum reflects internal structure of the particles. The hydrodynamic radii (DLS) were 2.5 nm and 310 nm in the unimer (low temperatures) and associated (high temperatures) state, respectively. These findings support the conclusion that the particles observed in dilute solutions cannot be identified with the core/corona micelles observed for solutions of amphiphilic copolymers in selective solvents.

The SANS experiments reveal that the particles formed by self-assembling of the X-shaped Tetronic macromolecules have multilayered internal structure (stacked lamellae, vesicles). Combination with the results of DLS and SLS techniques indicates that the particles are probably micron-sized multilamellar vesicles.

Their structure can be modified by mixing with POE/PPO copolymers with a simpler architecture (normal and reverse-type triblocks). For example, reverse-type triblock Pluronic RPE 1740 induces transition to unilamellar structure.

The structure evolution of the mixtures after temperature- and composition jumps were studied in time-resolved SANS experiments aimed at better understanding the equilibrium structures.

The thermosensitive copolymer structures were stabilized by adding sparingly soluble monomer (methyl methacrylate) and subsequent radiation-induced polymerization. This made it possible to study these structures by TEM.

DEMIXTION OF LIQUIDS IN A POROUS MATERIAL PROBED BY SANS

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The demixtion of a binary fluid mixture in confined media has been the object of several theoretical approaches both because of its fundamental aspects and because of the possible technical consequences. Experimentally, wetting properties and concentration fluctuations must be taken into account. SANS is an ideal method of observation because contrast variation allows the selective observation of each of the liquids in a porous matrix of silica. Results show that one of the liquids goes closer to the solid interface resulting in a very large liquid-liquid interface and a modification of the temperature dependence of the order parameter.

NEUTRON SCATTERING ILLUMINATES THE DYNAMIC STRUCTURES OF BIOLOGICAL MACROMOLECULAR COMPLEXES

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An important approach to the understanding of large macromolecular complexes under cellular conditions is via the study of environment effects (especially solvent composition and temperature) on their structures, interactions and dynamics. SANS plays an important role in such studies, because of contrast variation via solvent or component deuterium labelling, and the insensitivity of neutron absorption to very high solvent concentrations of salt, compatible, chaotropic and cosmotropic solutes. Where known, high-resolution structures of components from X-ray crystallography or NMR can be used in the interpretation. The method has been particularly fruitful for the study of protein-protein, protein-nucleic acid and lipid membrane-associated molecular machines. Recent and classical SANS studies in biology will be discussed as examples, including work on protein-RNA complexes of the protein translation apparatus, a light activated proton pump membrane protein, muscle protein function and the interferon cascade involved in resistance to viral infection [1-5].

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Posters

FIRST TESTS AND EXPERIMENTS WITH A NEW TYPE OF POSITION SENSITIVE DETECTOR IN SMALL-ANGLE AND BACKSCATTERING CONFIGURATIONS

A.I. Kuklin^*, S.A. Kutuzov*, A. Gabriel**, G. Eckold***, P.K. Utrobin*, A.A. Smirnov*, A.Kh. Islamov*, A.S. Kirilov*, A. A.Bogdzel and V.I. Gordeliy*

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The key element of a modernized YuMO spectrometer is a two detector system (TDS) [1,2]. The new setup of the instrument allows to collect simultaneously SANS data in a wide interval of scattering vectors. The momentum transfer dynamic range of the instrument has been considerably increased to more than 90 and data acquisition time has been reduced about two times. For the studies of anisotropic samples by TDS SANS spectrometer it is necessary to use PSD with a central hole. The idea of this detector was created by the SAS group of FLNPh and the detector was developed in a tight cooperation of the group with A. Gabriel and G. Eckold. The first tests of the detector with thermal neutrons have been performed at the G5-6 beam-line of LLB [3].

Here we report the experimental results which have been obtained in small-angle scattering as well as in diffraction (back scattering) modes at the YuMO instrument. The main parameters of the detector are as follows: the external size diameter -1070 mm; the size of the sensitive part of the detector is 580x580 mm^2; the detector comprises 230 wires with the 2.5 mm gap; the diameter of the central hole - 70 mm; the type of the position encoding - delay-line readout.

Finally the detector was placed into the detector vacuum tube of the YuMO and the experimental tests have been performed in the operational configuration of the instrument. It has been shown that the experimental scattering curves collected with the PSD and a standard YuMO circle detector are in agreement within experimental errors. The resolution of the detector is better than 3 mm. The data aqusition system is as fast as 1.7 Mevents/sec. It has been shown that the PSD with a central hole can be used for diffraction experiments in the backscattering mode as well.

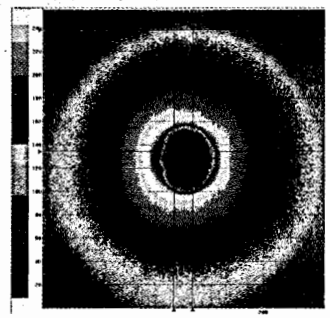

Fig.1 The small-angle neutron scattering picture for lipid membranes (log scale)

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Acknowledgements: We are grateful very much to A.Rogacev, A. Ivankov, A. Feoktistov, R.Erhan, Yu.Kovalev, T.Murugova, I.Ion, M.Balasoiu, A.Raevska; A.Churakov,V.Vasko, V.Comparat, A.Pelissier, J.Ballon, A.Mennel, M.Moon, A.N.Polyakov, G.Andreev, D. Kudryavtcev, E.Koberidze, G.Varenik, V.Ignatiev, A.Popov, A.Chernikov, V.Gaevskiy, V.Vstrechniy, A.Kurbakov, A.Balagurov, A.Beskrovniy, M. Kocsis, B.Guerard, G.Pepy, V.Sumin as well as to ILL, ESRF, LLB, ICC, EMBL staff for their generous help.

This work was supported by the Federal Ministry of Education and Science (BMBF) of Federal Republic of Germany under grant № 03DU03G2.

SOFTWARE COMPLEXES SONIX AND SONIX+: ELEVEN YEARS IN OPERATION

Kirilov A.S., Murashkevich S.M., Petukhova T.B.

The presentation is devoted to the history, main features and future prospects of software complexes Sonix and Sonix+, developed for instrument control. Since 1995 the 14 installations (together with its successor Sonix+) were made at neutron and x-rays instruments in Dubna (IBR-2) and Ekaterinburg.

The evolution of Sonix software was influenced greatly by the requirements of investigations at the SAS instrument. The Sonix was installed at YuMO at 1999. From the instrument control point of view the YuMO instrument is one of the most comprehensive instruments at the IBR-2 reactor. After studying the first operating experience, the complex was essentially redesigned. In order to achieve stable work, the structure of complex was changed:

- former X-clients were separated into "resident" and "interface" parts;
- the real time database (Varman from IRI TU Delft) was used for module communication;

Besides, the script control was appended with variables, loops, and other significant features. All these innovations were also used at other IBR-2 instruments.

In 2005 the two dimensional position sensitive detector has to be connected to the existing VME control system at YuMO instrument. The detector was handled by PC computer with Windows operating system. To connect a satellite PC to VME-based control system the method of combining Sonix and Sonix+ system was designed. This method has a device-independent protocol, it is easy to change or extend.

IMPROVEMENT OF TIME-OF-FLIGHT SMALL-ANGLE SCATTERING INSTRUMENTATION AND RESEARCH ACTIVITIES

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A modernization of the time-of-flight SANS YuMO spectrometer at the high flux pulse IBR-2 reactor (JINR, Dubna) was launched in 2000. The results which have been obtained with the new two detector YuMO setup, clearly demonstrate a remarkable progress in SANS instrumentation, which can be achieved by the use of a two or more detector system for registering scattered neutrons. Sample environment and sample preparation conditions for SANS studies were improved. Modernization of YuMO resulted in considerable increase of scientific activity at the instrument in the following directions: biology and biophysics, physical chemistry of surfactants and colloids, polymer physics and material science. The number of experimental proposals and publications have been increased considerably.

This work was supported by the Federal Ministry of Education and Science (BMBF) of Federal Republic of Germany and contribution from The Plenipotentiary Representative of Romania, Slovakia, Czechia, Poland at JINR.

SOFTWARE PACKAGE FOR TESTING AND DATA TREATMENT 2-D DETECTOR

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The new type of PSD ("Volga") with central hole was tested at low pressure (1.1 atm) at the beam-line G5-6 in LLB [1]. For the installation of the detector on the YuMO spectrometer new software package for control, tests and data treatment was done. We have shown the design and possibility of these programs, namely:

1)"Forsag" (program for preparation 1-D with TOFa data from 2D and TOFa data
2) 2DWR (program for work with detector on-line in all modes)
3)Tofa_2DWR_file (working with two-dimensional data)
4) N110_control
5) HV_Iseg_control
6) Sub_spec – program for subtraction files with coefficients.

This software package together with new "Sonix"software package [2] gives the possibility to all the advantage of TOF-method for "Volga" detector. High count rate (up to 2 Mevents/sec) and big size of data file (up to 128 Mb) set requirements of the software. These requirements have been successfully realized.

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This work was supported by the Federal Ministry of Education and Science (BMBF) of Federal Republic of Germany under grant № 03DU03G2.

MAGNETIC SYSTEM FOR SMALL ANGLE NEUTRON SCATTERING AT YUMO INSTRUMENT

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The small angle neutron diffractometer is widely used by colloid, polymer, biology scientists, other scientists involved in the investigation of nanomaterials and nanocomposites. A variety of auxiliary devices are necessary for complex studies of materials, in special environment conditions as: low and high temperature, high pressure, strong magnetic fields.

The new magnetic system constructed for YUMO instrument is presented (Fig.1). The magnetic system components are: the electromagnet with the goniometer, the power supply; computer for the automated command and control of the system.

The system was developed and constructed by the INCDIE ICPE CA Bucharest Romania in collaboration with CIPEC SRL Bucharest Romania.

The realization of the new position sensitive detector will permit the visualization and investigation of the magnetic field induced anisotropy in the analyzed sample.

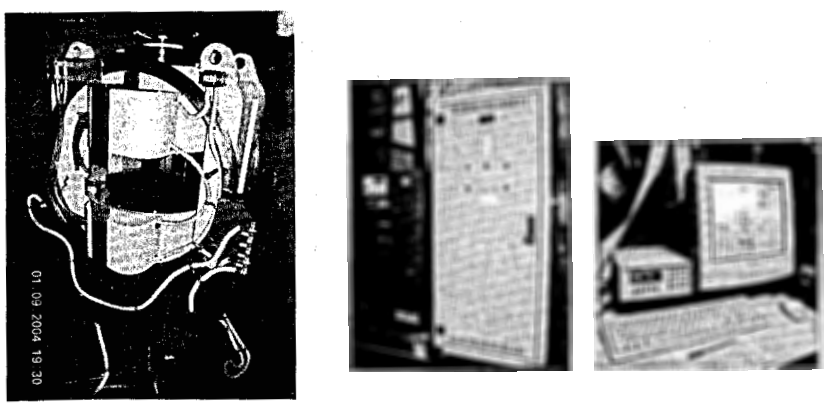

Fig1 Magnetic system for YUMO SANS instrument

Acknowledgements

We acknowledge the Governmental Romanian Plenipotentiary to JINR Dubna for the financial support through the JINR-INCDIE ICPE CA economic Contract Nr.08626319/021454-72.

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SMALL ANGLE NEUTRON SCATTERING INVESTIGATIONS OF MAGNETIC NANOFLUIDS BY MEANS OF CONTRAST VARIATION METHOD

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The diversification of carriers for producing ferrofluids enlarged the range of possible applications of these systems. The interest in obtaining good quality polar ferrofluids arises in connection with biological and medical applications. For example the magnetic fluid hyperthermia is a completely new approach for deep-tissue hyperthermia application because it couples the energy magnetically to nanoparticles in the target region. A further potential arises with magnetic nanoparticles generated for certain types of cancer, which are taken up selectively by malignant cells but not by normal cells of the same tissue type.

A principle possibility to use short chain length monocarboxylic acids (lauric and myristic acids) to stabilize magnetic nanofluids is reported. As a first step, these surfactants are used to coat magnetite nanoparticles in non-polar organic liquids, which results in highly stable magnetic fluids in respect to both the time factor and external magnetic field. The new fluids are compared with classical organic fluids stabilized by oleic acid, as well as with the less stable fluid with stearic acid.

The contrast variation technique in small-angle neutron scattering (SANS) experiments was applied to a new type of magnetic fluids based on organic non-polar carrier (benzene) and stabilized by myristic acid $C_{13}H_{27}COOH$ (surfactant from a series of monocarboxylic acids). The given surfactant differs much from the classical oleic acid $C_{17}H_{33}COOH$ used usually in such kind of solvents. It is shorter by four carbon groups and does not have a specific double bond in the middle of the molecule like oleic acid.

It was obtained the mean size of magnetite particles ~ 4.8 nm, which is almost two times less in comparison with the same parameter in the fluid with oleic acid (~8nm). Interesting thing is happened: while preparing the magnetic fluid, the kind of surfactant determines parameters of the size distribution function of the particles stabilized in the fluid!

This research project has been supported by the AEROSPATIAL research program of the Romanian Ministry of Education and Research, contracts OALM nr.111/2004, and TRAMAG nr.173/2004 and the grant of Governmental Romanian Plenipotentiary to JINR Dubna. M.V.Avdeev acknowledges the support from the INTAS Fellowship Grant for Young Scientists, Ref. N. 04-83-2582.

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INVESTIGATION OF RAT HEART MITOCHONDRIA BY SMALL ANGLE NEUTRON SCATTERING

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Low-amplitude matrix swelling stimulate specific structural reorganization. Namely so called "dried crista" have been detected in rat liver mitochondria [1]. They have small gap between ctista membranes. This structural changes are accompanied by rise of electron transport in respiratory chain, changes in pH-regulation of potassium transport and in kinetic parameters of oxidative phosphorylation [1,2,3].

The small angle neutron scattering (SANS) experiments with intact functioning rat heart mitochondria have been carried out on YuMO spectrometer (reactor IBR-2, JINR, Dubna) [4,5].

Mitochondria were placed in media containing 1 mM $MgSO_4 \cdot 7H_2O$, 1 mM KH_2PO_4, 20 mM *tris*, 10 mM *KCl*, 0.25 mM EDTA, 0.2 M sucrose (isotonic medium), 0.058 M and 0.028 M sucrose (hypotonic medium), pH=7.5. The temperature was 15 °C.

It has been shown that in case of isotonic medium mitochondrial crista form lamellar structures, which give peaks in scattering patterns with ratio positions of maximums 1:2. In case of hypotonic medium the curves have two peaks with the position ratio 1:1.3 and 1:1.6. that can indicate formation of non-lamellar structure (such as hexagonal and cubic [6,7]) by mitochondrial inner membrane. Such structural reorganization could greatly modify the functioning of mitochondrial enzymatic systems.

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INVESTIGATION OF INTERMEMBRANE INTERACTION IN PRESENCE OF DIMETHYLSULFOXIDE VIA SANS

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The present article is devoted to analysis of dimethylsulfoxide (DMSO) influence on the structure and intermembrane forces of dimyristoylphosphocholine (DMPC) lipid membrane using Small-Angle Neutron Scattering (SANS). The intermembrane spacing (D_w) was calculated at DMSO mole fractions X_{DMSO} up to 0.431 in gel and liquid phases at 12.5°C and 55°C, respectively. We have observed four typical regions in behavior of the repeat distance (D) that directly indicate at structural changes on lipid membranes. It was clear sown that thickness (D_m) of the lipid membranes does not change with increasing X_{DMSO}. The diffraction picture dramatically changes with increasing DMSO mole fraction. We have made a conclusion about membrane fusion when DMSO concentration was increased. Our calculation shown that DMSO penetrate extensively into the hydrophobic region of the lipid bilayers.

THE SPHERICAL CONE MODEL FOR SMALL ANGLE NEUTRON SCATTERING DENDRIMERS CURVES DATA TREATMENT

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A new spherical cone model (Fig. 1) has been suggested for treatment of the experimental data for the small-angle neutron scattering curves of G9Bu dendrimer. Two variants for four spherical cones are considered in the framework of this model. The mathematical justification of the model is discussed. Model's curves are represented for different values of the radii, the solid angles, and the density inside the dendrimer (Fig. 2). It is shown that this model fits the experimental data better than the ellipsoid model. The experimental and fitting curves are compared qualitatively. It is shown that only model with a solvent inside the dendrimer can be suitable for description of the experimental data. The proposed model is consistent with the previous experimental results [1], obtained with YuMO spectrometer [2].

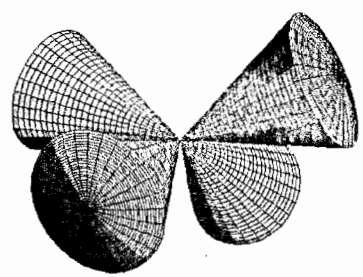

Fig. 1

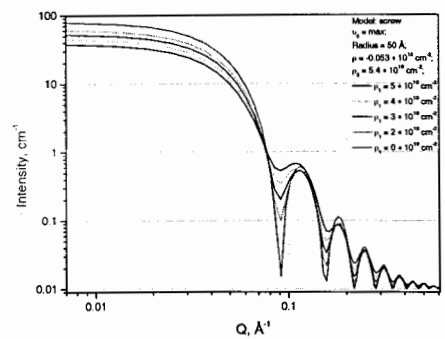

Fig.2

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PRECIPITATION OF TTAB/NABR MICELLES: THE EFFECT OF THE TEMPERATURE AND PRESSURE BY SANS AND VISUAL STUDY

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The behaviour of micellar solutions of tetradecyl-trimethylammonium-bromide (TTAB) has been investigated in a wide range of temperatures, pressures and electrolyte concentrations (NaBr) using the combination of small-angle neutron scattering and visual observations. It was shown that the liquid to solid phase boundary is shifted to higher temperatures and lower pressures by the addition of NaBr. Time-dependent experiments yielded that the kinetics of the transition into the solid phase is rather sluggish and occurs on a time scale of hours.

MOLECULAR ARCHITECTURE OF VIMENTIN INTERMEDIATES ASSEMBLY WITH SMALL-ANGLE X-RAY SCATTERING

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Intermediate filaments (IFs) together with microtubules and actin filaments, form the cytoskeleton of most living cells. IF assembly appears to be driven by a specific, hierarchic association of the elementary dimers in two directions: the lateral and the longitudinal. EM images of negatively-stained samples indicate that human vimentin repeated parts (ULFs - unit length filaments) are 16±3 nm wide and about 65 nm long [1].

The aim of the work presented here was to elucidate the detailed assembly pathway of human vimentin from tetramers to the ULFs, and to unveil the molecular structures of the corresponding intermediate oligomers. Here we employed SAXS to investigate the in vitro assembly of the wild-type human vimentin and a designed point mutant K139C.

At first, a qualitative study was made of gradual changing of the particle thickness i. e. of the lateral assembly of the dimers depending by external conditions with analysis of interatomic distance distribution function $p_{cr}(r)$ within the cross-section. Next, we built three-dimensional models of vimentin intermediates. Reliable construction of assembly intermediates models was only possible by a rigid body modelling method [3] complying with a number of sterical restraints deduced from the cross-linking results and other data. Solution conditions where a single oligomeric species (tetramer, octamer or 32-mer) was predominant, were found by a systematic screening of the measured data sets. Models of tetramer, octamer and ULF were constructed and refined based on dimer's structure taking into account additional structural restraints. We demonstrated that formation of tetramers, octamers and ULFs represent the principal steps along the vimentin assembly pathway. Next, the remaining non-monodisperse samples were represented as mixtures of the above vimentin intermediates. To determine the relative volume fractions of all oligomer types in every mixture the molecular models of tetramers, octamers and ULFs were further used. The results obtained in our study were further confirmed by electron microscopy and ultracentrifuge observations.

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FORMATION OF UNILAMELLAR PHOSPHATIDYLCHOLINE VESICLES PROMOTED BY Ca^{2+} IONS; CHANGES IN THE LIPID BILAYER THICKNESS

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Calcium ions have an important role in many cellular processes. The ions bind naturally to negatively charged phospholipids but rather weakly to zwitterionic lipids as phosphatidylcholine (PC) and phosphatidylethanolamine. We study the formation of unilamellar vesicles due to binding of Ca^{2+} ions to the saturated and monounsaturated PC bilayers, and the effect of ions on the lipid bilayer thickness. Dipalmitoylphosphatidylcholine (DPPC) or dioleoylphosphatidylcholine (DOPC) was hydrated in 0.2-60 mM solution of $CaCl_2$ in heavy water and thoroughly homogenized by freezing-thawing process. Small-angle neutron scattering (SANS) shows that calcium promotes the formation of PC unilamellar vesicles comparable to those prepared by extrusion. We detected formation of unilamellar vesicles already at 1 mM of $CaCl_2$ in the gel and liquid-crystalline phase of DPPC. From the Kratky-Porod plot $ln[I(Q)Q^2]$ vs. Q^2 of SANS intensity $I(Q)$ in the range of scattering vectors Q corresponding to the interval $0.001Å^{-2} \leq Q^2 \leq 0.006Å^{-2}$, the vesicle bilayer radius of gyration R_g and the bilayer thickness parameter d_g were obtained. With increasing concentration of Ca^{2+} ions, the lipid bilayer thickness of saturated DPPC shows changes in both, the gel and liquid-crystalline phase. The lipid bilayer thickness of monounsaturated DOPC (at 20°C) does not change in the concentration range 5-50 mM of $CaCl_2$. Differences in the area per 1 molecule of lipid in saturated and unsaturated PC can be responsible for observed effect.

Acknowledgements: The experiments were supported by the EC through NMI3, Contract n°: RII3-CT-2003-505925; by the JINR project 07-4-1031-99/2008, by the VEGA grant 1/3029/06, and by the APVV grant 51-027 404.

MOLECULAR MECHANISM FOR CONFORMATIONAL FLEXIBILITY OF RECA PROTEIN FILAMENT

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RecA protein is central enzyme in homologous DNA recombination, repair and other forms of DNA metabolism in bacteria. It functions as a flexible helix shaped filament bound on stretched single-stranded and double-stranded DNA. There have been mechanism proposed for the conformational transitions in DNA bound to RecA proteins. In this work we present atomic level model for conformational transitions of the RecA protein filament. The model describes small movements of the RecA N-terminal domain due to coordinated rotation of two main chain dihedral angles (/Lys23 and /Gly24) and preserves unchanged inter-subunit interface.

It is found that the model is capable to reproduce a wide range of observed changes of the helix pitch (83 - 101 Å) in transitions between compressed and stretched conformations of RecA filament observed by electron microscopy, atomic force microscopy and small angle neutron scatting (SANS).

Conformations of the helical filament in solution under varying conditions were studied by SANS on YuMO spectrometer (Dubna, Russia). The experimental and theoretical data indicate that the active conformation of RecA filament does not require DNA presence and that RecA protein can exist in a number of stable conformations with different geometric parameters of its filament structure. The conformational changes of RecA filament that result in the helical pitch increase are very well described by Lys23/Gly24 rotation. Changes in the filament radius of gyration cannot be explained by the mechanism, so that a sharp decrease of filament radius of gyration observed by SANS is to be attributed to other possible alterations in RecA protein conformation.

Grant support by the Russian Foundation for Basic Research grant 02-04-49259-a; Russian Academy of Science programs "Physics of Elementary Particles" (subprogram "Neutron physics", direction "Studies of structure,dynamics and nonordinary properties of matter by neutron scattering) and by the Ministry of Education and Science of Russian Federation grant RNP.2.2.1.1.4663.

LARGE-SCALE STRUCTURE OF RECA PROTEIN FROM DEINOCOCCUS RADIODURANCE IN SOLUTION

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Radiation resistant line of Deinococcus radiodurance exhibits unusual features in the regulation of post-radiation DNA degradation, homologous recombination and replication. The X-ray crystallographic structure of RecA from *D. radiodurance* exhibits usual for these proteins helical symmetry but with significantly lower helical pitch than seen in RecA protein from *E. coli* [1].

SANS measurements of the geometric parameters of the filaments formed by RecA protein from *D. radiodurance* in solution in different functional states were performed on YuMO spectrometer (Dubna, Russia). SANS scattering spectra of the protein self-polymer exhibited features characteristic for the helical filaments as seen in other RecA proteins [2,3]. In line with X-ray structure, the structure of the filament in solution was compressed with the pitch of the helix lower (approx. 60 Å vs 69 Å in *E. coli* protein) and the filament diameter somewhat higher than for *E. coli* protein.

Active filament (formed upon binding of DNA and ATPγS in the presence of Mg^{2+}) was characterized by increased helical pitch to 84 Å for the complex with ssDNA and 84 - 86 Å for the complex with dsDNA, as well as decreased mean filament diameter. Compared to RecA from *E. coli* and *P. aeruginosa*, filament formation on ssDNA required higher Mg^{2+}. At 2 mM Mg^{2+}, sufficient for formation of *E. coli* and *P. aeruginosa* filaments, RecA from *D. radiodurance* did bind to ssDNA, but the SANS spectra of such complex lacked a diffraction maximum characteristic for a helical structure. The filaments of RecA from *D. radiodurance* also required higher concentration of ATPγS (2.5 mM) to assume the active conformation. The filament geometry was dependent on the ionic strength of the solution, with the pitch increasing and the filament diameter decreasing in a buffer containing 1.8 M NaCl and showing continuous change in the geometric parameters of the filament at intermediate NaCl concentrations.

The study showed that RecA filaments from *D. radiodurance* can assume "open" and "closed" conformation, similar to those seen in other RecA proteins [2,3]. While inactive conformation is characterized by lower helical pitch and larger diameter of the filament than that of *E.coli* enzyme, the value for the helical pitch of the presynaptic complexes of this enzyme with ssDNA appears conservative. The geometry of the active complexes with DNA was very similar for ss- and dsDNA. It also appears that a variety of filament conformations are possible under conditions of elevated ionic strength, and at low Mg^{2+} concentration.

Grant support by the RFBR grant 02-04-49259-a; RAS program "Physics of Elementary Particles" (subprogram "Neutron physics", direction "Studies of structure, dynamics and nonordinary properties of matter by neutron scattering) and by the Ministry of Education and Science of Russian Federation grant RNP.2.2.1.1.4663.

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CONTRAST VARIATION IN SMALL-ANGLE SCATTERING EXPERIMENTS ON POLYDISPERSE AND SUPERPARAMAGNETIC SYSTEMS: BASIC FUNCTIONS APPROACH

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The development of the basic functions approach [1] for the contrast variation technique in the small-angle scattering from systems of polydisperse and superparamagnetic non-interacting particles is presented [2]. For polydisperse systems the modified contrast is introduced as the difference between the effective mean scattering length density (corresponding to the minimum of the scattering intensity as the function of the scattering length density of the solvent) and the density of the solvent. Then, the general expression for the scattering intensity is written in the classical way through the modified basic functions. It is shown that the shape scattering from the particle volume inaccessible for the solvent can be reliably obtained. Modifications of classical expressions describing changes in integral parameters of the scattering (intensity in zero angle, radius of gyration, Porod integral) with the contrast are analyzed. In comparison with the monodisperse case, the residual scattering in the minimum of intensity as a function of contrast (effective match point) in polydipserse systems makes it possible to treat the Guinier region of scattering curves around the effective match point quite precisely from the statistical viewpoint. But still, principle limitations of such treatment exist, which are emphasized in the paper. Also, the effect of magnetic scattering in small-angle neutron scattering from superparamagnetic nanoparticles is considered in the frame of the basic functions approach. Conceptually, modifications of the integral parameters of the scattering in this case is similar to those obtained for polydisperse multicomponent particles. Various cases are considered including monodisperse non-homogeneous and homogeneous magnetic particles, and polydisperse non-homogeneous and homogeneous magnetic particles. The developed approach is verified for two models representing the main types of magnetic fluids—systems of polydisperse superparamagnetic particles located in liquid carriers.

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20 YEARS OF TIME-RESOLVED WIDE AND SMALL ANGLE NEUTRON SCATTERING STUDIES AT THE IBR-2

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An experimental method of simultaneous accumulation of 8-dimensional neutron-sample interaction data has been proposed and used for the first time for understanding of any kind of radiation transfer through the matter on the basis of hydrodynamic mechanism.
Time-resolved wide and SANS experiments offered the possibility to generalize the interpretation of key phenomena in nature and to suggest the mechanism of self-organization of organic and inorganic matter, including massogenesis mechanism from chemical elements to cosmic objects, by harmonics and combination frequencies of resonance states.
A new organization of the experimental data about the dynamic state of the sample has been proposed.

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BALL SOLITONS AND KINETICS OF THE FIRST ORDER MAGNETIC PHASE TRANSITION (DISSIPATIVE STRUCTURES IN SPIN-FLOP TRANSITION)

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The theory of a new mechanism of the first order phase transition is presented. Magnetic ball solitons (BS) arise as the result of the energy fluctuations at the spin-flop transition induced by a magnetic field in antiferromagnets with uniaxial anisotropy. BS's are possible in a wide range of amplitudes and energy, including negative energy relative to an initial condition. When antiferomagnet is in a metastable condition, BS's are born with the greatest probability if the energy of solitons is close to zero. Evolution of these solitons, at which they develop into macroscopical domains of a new magnetic phase, leads to full phase reorganization. The birth of BS can be interpreted as occurrence of dissipative structures at the first order phase transition. Possible arrangements for experiments on the observation of elastic and inelastic scattering of neutrons by BS's are shown.

INVESTIGATION OF POLYMERIC RUBBER BY SANS

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The preliminary results about the influence of the sulphur concentration vulcanized during the polymerization process into polymeric rubber (polybutadiene) (1.1% - 2.8% sulphur in rubber) was studied by SANS (small-angle neutron scattering) with YuMO spectrometer [1] at IBR-2 pulsed reactor of JINR, Dubna.
The experiment was performed at room temperature. It was shown that the correlation peak corresponds to a 130 Å size of inhomogeneity and presents a weak dependence from concentration of sulphur.

[1]A.I. Kuklin, A.Kh. Islamov, V.I. Gordeliy, Two-Detector System for Small-Angle Neutron Scattering Instrument, Neutron News, vol.16, Issue 3, 2005

SANS CONTRAST VARIATION ON MAGNETIC FLUID STABILIZED BY SHORT CHAIN LENGTH MONOCARBOXYLIC ACID

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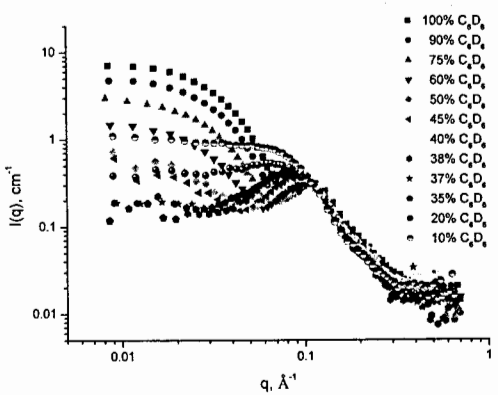
The contrast variation technique in small-angle neutron scattering (SANS) experiments was applied to a new type of magnetic fluids based on organic non-polar carrier (benzene) and stabilized by myristic acid $C_{13}H_{27}COOH$ (surfactant from a series of monocarboxylic acids). The given surfactant differs much from the classical oleic acid $C_{17}H_{33}COOH$ used usually in such kind of solvents. It is shorter by four carbon groups and does not have a specific double bond in the middle of the molecule like oleic acid. The small-angle neutron scattering (SANS) investigations of magnetic fluids were carried out with the time-of-flight small-angle-scattering spectrometer YuMO [5] at the IBR-2 reactor of JINR.

Scattering curves obtained at the YuMO instrument for samples with the 0.86 % volume fraction of magnetite and different relative content η of deuterated component in the carrier (benzene) are given:



From the scattering curves the mean size of magnetite particles was determined (~4.8 nm), which is almost two times less in comparison with the same parameter in the fluid with oleic acid (~8 nm). Possible explanation is given.

[1] M.Balasoiu, M.V.Avdeev, A.I.Kuklin, V.L.Aksenov, D.Bica, L.Vekas, D.Hasegan, Gy.Torok, L.Rosta, V.Garamus, J.Kohlbrecher, *Magnetohydrodynamics* **40** (2004) 359-368
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SANS STUDY OF STRUCTURAL CHANGE OF THE COAL-TAR-PITCH DERIVATIVES INDUCED BY CARBON NANOTUBES ADDITION

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The analysis of SANS-data from coal tar pitch carbonized at 460^{0}C with addition of 1.5 wt. % single and multiwalled nanotubes (SWNT and MWNT) is reported. A structural model consisting of two structural levels was proposed as result of SANS-data and classical interpretation of carbon structure [1, 3]. As a structural feature, the first level presents the clusters with surface fractal properties and diameter not less then 800 Å. The second level consists of the basic structural units (BSU), which form the inner part of the first level. The type or/and size of the additives have a key role in the development of the structure at this length scale.

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SANS DATA TREATMENT SOFTWARE

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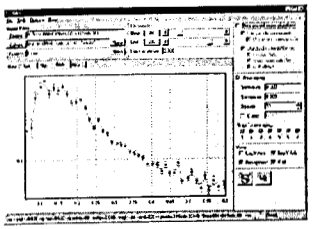
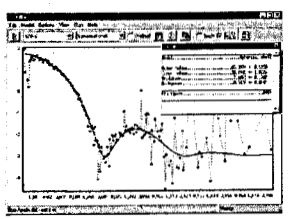
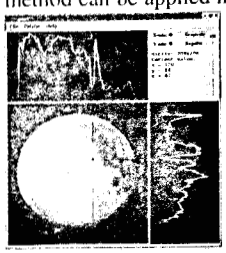
The main two steps - primary and secondary ones - of in small angle neutron scattering data processing are performed with the help of SAS and Fitter packages correspondingly.



The SAS [1] program is aimed to process the spectra measured on YuMO spectrometer (channel four of the IBR-2 reactor). The program allows to combine the data referring to the same sample, to calculate the spectrometer resolution function for the given experiment conditions, to carry out data correction on dead times of neutron detectors, and to subtract a background substrate from detector data (in two possible modes: using the neutron beam breaker or without it), to carry out the normalization of the obtained spectrum on standard vanadium scatterer, to subtract background sample data.

Fitter [2] is a C++ program aimed to fit a chosen theoretical multi-parameter function through a set of data points. The method of fitting is chi-square minimization. Moreover, the robust fitting method can be applied in Fitter. Fitter was designed to be used for a small-angle neutron scattering data analysis. Respective theoretical models are implemented in it. Some commonly used models (Gaussian and polynomials) are also implemented for wider applicability.

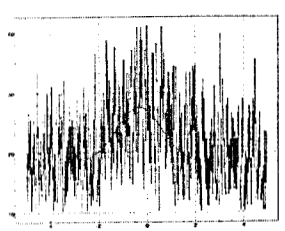


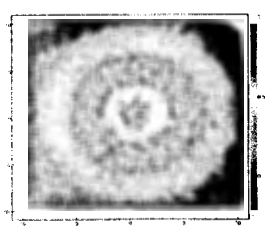


SAS is based on the Histogram Template Library (HTL) [3]. It is a C++ class library that provides basic functionality for one-dimensional histograms. As the name suggests, it exploits the template facility of C++ and is designed to be easy to use, compact and performant.

Both SAS and Fitter packages are used RC [4] - a kit of C++ classes that provides functionality for easy to use management of runtime configuration parameters, for storing them in configuration file.

One more package should be mentioned is MaVi [5] (MAtrix VIewer) is s simple visualization program for matrix data. Data is displayed inside the main window as 2D color field and two orthogonal 1D slices can be chosen in additional windows. MaVi allows one to pick up and explore the individual elements of the matrix. It can be used for on-line or off-line analysis in the control or data acquisition systems.





Finally, one useful standalone package – Gluplot [6] - appears during SANS software development. Gluplot is a data plotting package. It was originally

intended both as graphical library and as standalone program which would allow scientists and students to visualize data. (The "GLU" in gluplot means that it is OpenGL/GLU/glut based.) Gluplot handles both curves (2D) and surfaces (3D). For 2D plots, there are many plot styles, including lines, points, lines with points, error bars and impulses. Surfaces are plotted as a color map on the x-y plane. Gluplot supplies both linear and logarithmic axes. Moreover, any other axis distortion is available using gluplot library. Axis scale and also many other settings are changeable by gluplot command-line options or by menu items and hot-keys after it runs. After all, gluplot supports high quality plot output to PostScript (PS), Encapsulated PostScript (EPS) and Portable Document Format (PDF) files.

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[6] http://www.jinr.ru/programs/jinrlib/gluplot/indexe.html

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Научное издание

International Small-Angle Scattering Workshop devoted to the 70th anniversary of Yu. M. Ostanevich's birth

Programme and Abstracts of the Workshop

Международное совещание по малоугловому рассеянию, посвященное 70-летию со дня рождения Ю. М. Останевича

Программа и тезисы докладов

E13,14-2007-53

Сборник отпечатан методом прямого репродуцирования
с предоставленных оригиналов.

Ответственный за подготовку сборника к печати *А. И. Куклин.*

Подписано в печать 22.05.2007.
Формат 60 × 90/16. Бумага офсетная. Печать офсетная.
Усл. печ. л. 3,75. Уч.-изд. л. 4,73. Тираж 200 экз. Заказ № 55778.

Издательский отдел Объединенного института ядерных исследований
141980, г. Дубна, Московская обл., ул. Жолио-Кюри, 6.
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