XII INTERNATIONAL CONFERENCE ON SELECTED PROBLEMS OF MODERN PHYSICS

Dedicated to the 95th anniversary
of the birth of D. I. Blokhintsev
(1908–1979)

Section II
Physical Investigations at Pulsed Reactors

Programme and Abstracts

Joint Institute for Nuclear Research

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Dedicated to the 95th anniversary of the birth of D. I. Blokhintsev (1908–1979)

Dubna, Russia, June 8–11, 2003

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Physical Investigations at Pulsed Reactors

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Dubna 2003

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11.00		**Coffee**	**Coffee**	**Coffee**	11.00
11.30	**Memorial Session dedicated to D.I.Blokhintsev**	**Parallel Sessions:** "Cold Moderators", "Neutron Instrumentation and Methods", "Neutron Physics"	**Parallel Sessions:** "Biology and Polymers", "High Pressure Physics and Earth Sciences", "Neutron Physics"	**Parallel Sessions:** "Complex Solutions", "Materials Science", "Neutron Physics"	11.30
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8 June (Sunday)

Blokhintsev Laboratory of Theoretical Physics, JINR

10.30 **Registration**

11.00 **Memorial session dedicated to D.I.Blokhintsev**

V.G.Kadyshevsky, A.A.Logunov, E.P.Shabalin, A.N.Sissakian, V.I.Trukhin, A.V.Zrodnikov

13.00 **Lunch**

Dubna Branch of the Skobeltsyn Institute of Nuclear Physics of MSU

Plenary Session

15.00 V.L.Aksenov
"IBR-2 Reactor in XXI Century"

15.30 A.V.Gulevich
"Concept of Laser System Pumping with IBR - Type Reactor"

16.00 **Coffee**

16.30 S.V.Vorontsov
"RFNC-VNIIEF Pulse Reactors Design and Operation Experience"

17.00 K.Clausen
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17.30 V.S.Barashenkov
"From Obninsk to Dubna -How to Combine Atomic Reactor with Accelerator?"

9 June (Monday)

Dubna Branch of the Skobeltsyn Institute of Nuclear Physics of MSU

Plenary Session

09.00 V.N.Shvetsov
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09.30 L.B.Pikelner
"About Nature of the Parity Violation Effect at the Interaction of Neutrons with Lead Isotopes"

10.00 H.Lauter
"Ability of Polarised Neutron Reflectometry to Study Artificial Magnetic Structures"

10.30 Th.Rekveldt
"Neutron Spin-Echo for SANS and Reflectometry"

11.00 **Coffee**

Parallel Sessions

Session "Cold Moderators"

11.30 Yu.Ya. Stavisski
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11.50 E.P.Shabalin
"Conception of Cold Moderator with Solid Aromatic Hydrocarbons"

12.10 H.Tietze-Jaensch
"The ESS Moderator Concept and Instrument Layout of the Short Pulse and Long Pulse Target Stations"

12.30 Y.Kiyanagi
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12.50 H.Conrad
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13.10 **Lunch**

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15.20 I.Natkaniec
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"Radiation Properties of Prospective Moderator Materials"

16.00 **Coffee**

Session "Complex Solutions"

16.30 M.Balasoiu
"Structural Studies of Ferrofluids by Small-Angle Neutron Scattering"

16.50 G.Klose
"Determination of Multilamellar Vesicle Portions in Extruded Phospholipid Dispersions by SANS"

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Session "Neutron Instrumentation and Methods"

11.30 A.M.Balagurov
"Ultra-High Resolution Neutron Diffraction Using Fourier Chopper Technique"

11.50 Ch. Scheffzük
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"A Comparison of Different Methods for Improving Flux and Resolution on TOF-SANS Instruments"

12.30 A.I.Kuklin
"The Modernized Small-Angle Neutron Scattering Spectrometer YuMO"

12.50 D.V.Sheptyakov
"Direct Structure Determinations From HRPT Neutron Powder Diffraction Data"

13.10 **Lunch**

15.00 V.B.Zlokazov
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15.20 V.N.Shvetsov
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15.20 S.P.Melnikov
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15.40 S.L.Turutin
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16.00 **Coffee**

16.30 Yu.A.Alexandrov
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16.50 S.V.Borzakov
"Experimental Possibilities to Investigate the Nucleon-Nucleon Interaction in the Low Energy Region"

17.30 **Poster session**

"Cold Moderators",
"Neutron Instrumentation and Methods",
"Condensed Matter Physics-1"

10 June (Tuesday)

Dubna Branch of the Skobeltsyn Institute of Nuclear Physics of MSU

Plenary Session

09.00 Yu.A.Izyumov
"Dynamics of Longitudinal Components of Isotropic Ferromagnet"

09.30 A.R.Khokhlov
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10.00 S.M.Stishov
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10.30 M.V. Frontasyeva
"FLNP JINR Contribution to the European Programme "Atmospheric Heavy Metal Deposition"

11.00 **Coffee**

Parallel Sessions

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11.50 L.S.Yaguzhinsky
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12.10 A.I.Kuklin
"Investigation of Polymers by Neutrons on IBR-2"

12.30 A.S.Andreeva
"Small Angle Neutron Scattering Study of the Influence of the Nature of Bond Between Hydrophilic Backbone and Hydrophobic Side Chains on the Structure of Hydrophobically Modified Gels"

12.50 G.Pepy
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13.10 **Lunch**

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15.20 V.V.Isaev-Ivanov
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15.40 D.V.Lebedev
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16.00 A.Kh.Islamov
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16.20 A.Kh.Islamov
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16.40 *Brief Oral Presentations of Posters of Young Scientists*

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Session "High Pressure Physics and Earth Science"

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15.00 V.V.Sikolenko
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15.40 T.I.Ivankina
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16.00 A.N.Vinogradov
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16.20 Yu.P.Smirnov
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11.50 V.F.Kolesov
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12.10 V.F.Kolesov
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17.00 **Poster session**

"Condensed Matter Physics-2",
"Neutron Physics",
"Neutron Activation Analysis for Life Sciences"

11 June (Wednesday)

Dubna Branch of the Skobeltsyn Institute of Nuclear Physics of MSU

Plenary Session

09.00 N.M.Plakida
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09.30 R.Blinc
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10.00 H.Fuess
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10.30 I.G.Smirnov
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11.00 **Coffee**

Parallel Sessions

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12.20 A.V.Tamonov
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12.40 K.Walther
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13.00 S.I.Morozov
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13.30 **Closing**
14.00 **Lunch**
16.00 **Steamer Voyage**

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9 June (Monday)

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M-4 H.Tietze-Jaensch
The European Spallation Source Facility. Instruments and Layout

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I-3 P.K.Utrobin
"Installation of High Hydrostatic Pressure on Small-Angle Spectrometer YuMo"

I-4 E.A.Raitman
"Inelastic Neutron Scattering on Acoustic Waves in Solids Studied by NSE"

I-5 V.N.Gavrilov
"Neutron Reflection from an Ultrasonically Excited Layered Structures and Glass Mirror"

I-6 V.N.Gavrilov
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CM1-3 I.Ion
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CM1-4 L.Almasy
"Characterising of Local Order in Aqueous Surfactant Solutions by SANS and Thermodynamic Methods"

CM1-5 O.V.Sobolev
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CM1-6 S.N.Bushmeleva
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CM1-7 A.E.Sokolov
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10 June (Tuesday)

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CM2-3 S.E.Kichanov
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CM2-13 L.S.Smirnov
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CM2-14 L.S.Smirnov
"The Study of Ammonium Ion Dynamics in the $K_{1-x}(NH_4)_xCl$ Mixed Crystals"

CM2-15 S.A.Danilkin
"Lattice Dynamics of Hydrogenated Austenitic Steels"

CM2-16 V.Rajevac
"Lattice Dynamics in Austenitic Stainless Steels"

CM2-17 S.I.Morozov
"Determination of the Hydrogen Content in Constructional Materials by Slow Neutron Scattering Methods"

CM2-18 A.V.Knotko
"The Small Angle Neutron Scattering on the Extensive Defects in the Pr - Substituted $Bi_2Sr_2CaCu_2O_8$"

CM2-19 Yu.D.Zaroslov
"Self-Assembly of Polyelectrolyte Rods in Polymer Gel and in Solution: Small Angle Neutron Scattering Study"

CM2-20 D.Uhrikova
"SANS and SAXD Study DNA+DOPC+Ca^{2+} Aggregates"

CM2-21 D.Uhrikova
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CM2-23 Yu.S.Kovalev
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NP-1 V.Pronyaev
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NP-2 V.Pronyaev
"Quantification of Data Uncertainties"

NP-3 *R.U.Khafizov*
"Search for Radioactive Beta-Decay of the Free Neutron"

NP-4 Yu.V.Ryabov
"About Stability of a Gamma-Registrations for Ge(Li)-Detectors at Long Time Intensive Radiation"

Session "Neutron Activation Analysis in Life Sciences"

NA-1 N.G.Aksenova
"Neutron Activation Analysis of Mercury in Spirulina Platensis Used as a Sorbent"

NA-2 T.E.Galinskaya
"Heavy Metal and Rare Earth Elements Distribution in the Different Components of Rybinsk Reservoir Ecosystem"

Abstracts

Plenary Talks

D.I.BLOKHINTSEV – THE FIRST SCIENTIFIC DIRECTOR OF THE LABORATORY "V" (TO THE BIOGRAPHY OF D.I.BLOKHINTSEV, 1950-1956)

A.V. Zrodnikov, Yu.V. Frolov

SSC RF Institute for Physics & Power Engineering
1, Bondarenko Sq., Obninsk, Russia 249020

This report is dedicated to the activity of D.I.Blokhintsev at the post of the Director of the Laboratory "V" (now - SSC RF Institute for Physics & Power Engineering in Obninsk) in 1950-1956 years.

D.I.Blokhintsev is one of the leaders of Institute for Physics & Power Engineering, at the time of its foundation, along with such famous physicists as Academician of the Ukrainian Academy of Sciences A.I.Leipunski and Academician of the Academy of Sciences of Belarus A.K.Krasin. He become the first Director-scientist changed at this post directors-builders and administrators appointed from the officers personnel of the Ministry of Internal Affairs of the Soviet Union.

He headed the Institute at the critical moment of its history. Namely, in this period the main scientific directions of the research in the Institute for Physics & Power Engineering has been formed. Most of these directions remain actual at the present time.

In the report the principal role of D.I.Blokhintsev as

- The Leader of the starting up of the first physical assembly of the uranium-graphite reactor in the Institute (1954);
- The scientific Leader of the development and starting up the first atomic power station in the world (1951-1954);
- The scientific Leader of the calculation-theoretical investigations for the creation of the first thermonuclear explosive device, which were carried out in the Laboratory "V" in 1951-1955;
- The Leader of the research and development investigations for the creation of transport reactors and fast neutron reactors;
- The main author of the ideology of the development of the pulsed reactor with periodical action.

An attempt is made to give a picture about the position of D.I.Blokhintsev in the questions of the theoretical physics state in the USSR in that years and problems of its development, his assessments of the state of the nuclear forces theory and his relationship to the ideological discussion about the role of physics in the society.

HISTORY OF CREATION OF PULSED REACTORS

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IBR-2 REACTOR IN THE XXI CENTURY

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The present status and trends of the development program of the IBR-2 reactor are discussed. The special attention is drown to a new conception of the moderator complex around new reactor IBR-2M. The strategy of research programs and instrumentation developments is considered.

IBR-2 modernization work schedule

IBR-2 operation for physical experiment	2004-2006
MR-3 startup	2003
Creation of fuel loading for IBR-2M	2005
Development of design documentation	2004
Production of major IBR-2 equipment: Jacket, roll-away shielding, stationary ferlectors, CES mechanisms	2006
Development and production of CES electronics	2008
Construction of cryogenic helium station for CM	2005
Development and production of new moderators for IBR-2	2007
Upgrading of technological equipment	2003-2008
Dismantling of IBR-2 used-up equipment	2007-2008
Assembly and adjustment of new IBR-2M equipment	2008-2009
IBR-2M physical startup	2009

IBR-2M parameters:

Mean power	2 MW
Neutron flux	$2.4 \cdot 10^{16}$ n $cm^{-2} s^{-1}$
Fast neutron pulse width	200 μs

The result of the modernization is that JINR will have operating the only pulsed neutron source of the world class of all the JINR Member States. Its parameters will be unique in many aspects, which will make it possible for IBR-2 to remain one of the best neutron sources for physical research for another 20 – 30 years after 2010.

CONCEPT OF LASER SYSTEM PUMPING WITH IBR TYPE REACTOR

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Nuclear pumped lasers are driven by the nuclear reaction products providing the direct conversion of nuclear energy to optical energy.

One of the most perspective conceptual design of the high power reactor pumped laser system based on the optical quantum nuclear reactor-pumped amplifier (RPA) had been proposed in the Institute of Physics and Power Engineering several years ago [1].

RPA is a coupled reactor system consisting of pulse periodic fast reactor and deep-subcritical (in neutron sense) laser module (LM) with the multiplication factor ~ 0.8 – 0.9. Reactor and laser modules are principal components of RPA. Periodic pulsed fast reactor [2] is equipped with a liquid metal cooling system of the active core. If necessary a several pulsed reactors can be used. LM acts as a multiplier of reactor neutrons. It is shaped as a cylindrical structure sized to provide the space for housing the active core and reactivity modulator of pulse reactor. The pumping section of the laser module is filled with a gaseous or liquid laser active medium containing a fissile material and includes the elements of a neutron moderator. This section is surrounded with reflector of neutrons, flanks are prepared from an optically transparent material to provide the input and output of the laser beam. The fission energy of uranium in the laser module can be utilized for pumping of laser. The liquid metal coolant system may be used to remove the surplus heat energy from the LM.

The energy demo model of a pulse nuclear reactor pumped laser system on the base of the two core "Bars-6" fast burst reactor [3] is created at IPPE. It was started up in 1999.

This report is devoted mainly to the analysis of the neutron characteristics of the coupled reactor system «periodic pulsed reactor – subcritical module» and the experimental results received during the energy start-up of the system. Comparative analysis for computed and experimental neutron data is performed.

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RFNC-VNIIEF PULSE REACTORS DESIGN AND OPERATION EXPERIENCE

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The neutron-physical laboratory for preparing and carrying out experimental measuring of first РДС-type nuclear bombs was established under direction of G.N. Flerov in 1948 at KB-11 in Sarov.

The line of works related to performance of criticality experiments was constantly being in progress at VNIIEF. There were developed special stands for critical assemblies (SCA), whose design was improved, while accumulating the experience (FKBN, FKBN-1, MSKS, FKBN-2, FKBN-2M), there were manufactured unified sets of hemispheric parts made of fissile and inert materials. During the last period there were studied parameters of ~1000 different multiplying systems (MS). At present FKBN-2M facility is being intensely used to conduct different experiments related, in particular, to development of nuclear power engineering and neutron constants improvement /1,2/.

Since the 1960s VNIIEF's specialists have been searching for ways of creating powerful laboratory pulse neutron sources (pulse nuclear reactors - PNR) capable to simulate penetrating nuclear explosion radiation. The neutron fluence per pulse, the volume of space available for irradiation with high fluence, and the pulse duration were taken as basic characteristics of PNR (as a source of ionizing radiation). In this case one tried to make the first two characteristics possibly maximal, and the third one - minimal /1,3,4/.

The wish to attain high intensity of energy release in the core led to the necessity of solving the problem of thermal shock effect in PNR fuel cells decreasing. Intention to obtain intense fields of ionizing radiation in large volumes stimulated application of new materials for pulsed reactors fuel cells. The mentioned works have led to developing of the unique park of pulsed nuclear reactors operating both autonomously and as a part of irradiation complexes involving powerful pulsed electron accelerators of LIU type /1, 3-5/.

At present 6 PNR are operating at VNIIEF /1,3,4/:

- PNR with metal core - BIR-2M, BR-1, BR-K1, GIR -2;
- PNR with ceramic core - BIGR;
- PNR with solution core - BIR-2M.

During operation there have been generated over 10,000 prompt bursts by the various reactor types and lots and lots of different researches have been carried out including radiation hardness, nuclear pumping lasers, fuel behavior during RIA accident, ultra-cold neutrons production etc. /1/

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THE EUROPEAN SPALLATION SOURCE ESS, A VISIONARY TOP CLASS PULSED NEUTRON FACILITY TO EUROPE'S LEADERSHIP IN SCIENCE USING NEUTRON BEAMS

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The European Spallation Source ESS is a proposed top tier facility for European science using pulsed neutron beams. A consortium of 18 European laboratories from 11 countries worked out a technically feasible project proposal that was well recognized among the global science community and that would maintain Europe's lead in all fields of science and technology using pulsed neutron beams. Politics acknowledged the project and recognized the long term need in Europe for a facility like ESS. However, recent political decisions in Germany were not to support ESS is the short term. The ESS council has therefore decided to take appropriate actions to adapt and slow down the technical development work on realizing the project, but also to maintain its visibility in science, society and politics and to keep it alive, i.e. permanently recoverable.
The scientific potential of condensed matter research using neutrons as a highly competitive and complementary probe is presented. ESS project visions and its scientific missions are mentioned and various scenarios of an eventual realization of ESS are discussed.

FROM OBNINSK TO DUBNA - HOW TO COMBINE ATOMIC REACTOR WITH ACCELERATOR?

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Today only few people know that the famous center of atomic power engineering in Obninsk began with design of various types of powerful accelerators and D.I.Blokhintsev, who became afterwards a director of this center and a builder of the first atomic power plant, took an active part in calculating the trajectories of particles in electromagnetic fields. He kept his interest in combining two basic atomic machines - an accelerator and a nuclear reactor - up to the end of his life. His move to Dubna opened splendid possibilities for realization of this idea.

Here in the middle of the 60s, V.I.Gokdamsky's group performed experiments with a huge, 20 tons Uranium slab on the proton beam of 660 MeV phasotron. The neutron yield was so large that it allowed one to consider seriously the old Lourens and Semenov's idea about the use of a high-current accelerator for the transmutation of Uranium into easy-fusible Plutonium. Since the subsequent experiments were complicated and costly, D.I.Blochinsev proposed to use mathematical modeling instead them. LTP and LCTA, JINR, under his leadership the development of the theory of intra- and internuclear cascade, designing of software and mathematical experiments with various types of electronuclear reactors started. It was 40 years ago.

In the beginning of the 70s P.L.Kirillov organized in Obninsk an "electronuclear seminar" convoking physicists from many institutes of the former Soviet Union. The result of several sessions of this seminar was a Proposal sent to the responsible for atomic technology Ministry "Sredmash" about more intensive investigations in this area. The Proposal has been approved and Moscow ITEP was selected as a head center. JINR the electronuclear investigations concentrated in LHE and LCTA. Several months before his sudden death D.I Blokhintsev discussed with me and K.D.Tolstov the perspectives of this branch of nuclear technology and plans of the future investigations. In particular, various possibilities to decrease the beam intensities in electronuclear systems what still remains as a main problem.

One should note that the main goal of the electronuclear investigations at that time was the production of the largest volumes of weapon grade Plutonium. A principal alteration of the strategy has been done after the "cold war" by Carlo Rubbia suggested a scheme "one accelerator - one reactor" with the use of the produced Plutonium and the transmutation of radioactive waste into short-living ones. Such subcritical and safe energy generators and wast transmutators demand only about 10 -30 mA accelerator current what is in limits of the modern technical ability.

Perspectives of the electronuclear technology will be considered, several of which were already discussed by D.I.Blockintsev: use of Thorium fuel, deuteron and high-energy heavy ion beams, multireactor accelerator driven systems, the combined use of several accelerators with energies of hundreds MeV and so on.

ABOUT NATURE OF THE PARITY VIOLATION EFFECT AT THE INTERACTION OF NEUTRONS WITH LEAD ISOTOPES

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The effect of parity violation in lead was firstly found by B.Heckel et al. [1] when authors were observing spin rotation of polarized thermal neutrons passing through the natural lead target. The absence of s- and p-resonances near the "thermal point" makes the explanation of this effect a difficult task. Further, it was experimentally shown by O. Ermakov et al [2] that the effect is connected with the isotope of ^{204}Pb. However, it did not answer the question because it requires the presence of very strong "negative" resonance near the "thermal point". The measurements of dependence of radiative neutron capture cross section on energy can be used to found such resonance. This dependence differs very much for s- and p-waves.

Such measurements are being carried out on pulse neutron source IBR-2 by means of COCOS device, which includes combination HPGe detector and BGO scintillators. Energy dependence of the cross section is being observed by means of registration of gamma-quanta of direct transition from the excited state of compound nucleus to the ground state.

As a result of the measurements there was discovered that appropriate negative resonance is at ^{207}Pb isotope, but not at ^{204}Pb. So it's most probably that ^{207}Pb isotope determines the parity violation effect in natural lead.

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ABILITY OF POLARISED NEUTRON REFLECTOMETRY TO STUDY ARTIFICIAL MAGNETIC STRUCTURES

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The unique abilities of polarised neutron reflectometry (PNR) are best outlined under the expression of "layer selective magnetometry". Indeed, PNR provides the information about magnetisation vector depth profile of artificially created magnetic superstructures of scientific and technological importance. Studies of antiferromagnetically exchange coupled multilayers, biased multilayers, etc will be presented.

Rather recently the structural information also along the surface direction including their perpendicular distribution became accessible, which arise e.g. from artificial gratings, magnetic domains or interface roughness. Even more important is the progress made in the theoretical description of the measured events in off-specular scattering directions. Grazing incidence diffraction or small angle scattering is complementary in view of the length scale.
A further step to reach 3-dimensional polarimetry is possible in a special set-up to investigate also the perpendicular to the surface magnetic moments.

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NEUTRON SPIN-ECHO FOR SANS AND REFLECTOMETRY

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Neutron spin-echo uses the Larmor precession of the neutron spin to label each neutron with its wavelength and transmission angle. Measuring the deviation form echo in two identical precession devices gives information about the change in wavelength and/or transmission angle. Up to recently this technique was only used for energy analysis by studying the change in wavelength. More recently the technique was applied also for measuring the change in transmission angle very accurately [1]. With the precession regions in parallel mode very high-resolution diffraction could be carried out. In this presentation the use of the technique for SANS and reflectometry will be explained in some detail. The application in SANS appears to be equivalent with measuring in real space. The application in reflectometry enables one to measure the Q-dependent reflectometry with very high accuracy, independent of beam divergence and sample waviness.

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DYNAMICS OF LONGITUDINAL COMPONENTS OF ISOTROPIC FERROMAGNET

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In the beginning we give a review of theoretical and experimental study of dynamics of a Heisenberg ferromagnet in a wide temperature interval except a critical region. The basic dynamical modes of transversal spin components are spin waves, which are well defined at small enough wave vectors up to the Curie point. Theory and experimental data on inelastic neutron scattering are in good agreement each other.

The other thing is dynamics of longitudinal spin components. Since a paper [1] it was clear that their dynamics is determined by processes of virtual absorption and emission of spin waves, which increase very much at high temperatures. However many theoretical attempts to construct the proper theory were contradictive. The reason for the theoretical difficulties is strong nonlinearity in the dynamics of longitudinal components. Experiments with inelastic neutron scattering gave also contradictive results on longitudinal spin susceptibility. In some experiments two -peak structure was observed for dynamical structure factor, in others one wide maximum centered at zero energy was found.

Recently we used for study of this problem a diagrammatic technique for spin operators, developed by us in 1968. In framework of this technique we summed up infinite series of loop-type of diagrams , formed by renormalized spin waves, and calculated dynamical longitudinal susceptibility [2-4]. The dynamical structure factor in general case has a three-peaks structure. Along with two wide maxima , corresponding to damped wave modes a not narrow central peak appears. Its intensity grows when approaching to Curie point. In result all three peaks can merge and create a wide frequency distribution. Position of the wide peaks and their width change linearly with wave vector q. Thus depending on parameters of a system and on temperature one may observe either three- peak structure or a wide maximum in dynamical structure factor of longitudinal fluctuations. It may explain contradictive results of neutron scattering experiments.

Our theory is applicable beyond hydrodynamic regime that is valid at small q and higher temperatures. Suggested generally three-peak structure is in qualitative agreement with resent Monte-Carlo calculations for classical Heisenberg ferromagnet [5].

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STRUCTURE OF AMPHIPHILIC POLYMER HYDROGELS AS REVEALED BY NEUTRON SCATTERING

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Amphiphilic polyelectrolyte hydrogels of copolymers of acrylic acid and n-alkylacrylate being immersed in aqueous media undergo self-organization with the formation of hydrophobic domains. For most of uncharged gels a scattering peak is observed. It is attributed to the correlation between hydrophobic domains formed by self-assembled n-alkyl side chains. From the SANS data the aggregation number of the hydrophobic domains was derived. It was shown that it increases with increasing length of hydrophobic groups and also as a result of absorption of hydrophobic additives that are solubilized inside hydrophobic domains.

The most important observation of this work consists in the fact that the introduction of charged groups into the gel leads to microphase separation with the formation of periodically arranged hydrophobic regions including several densely packed hydrophobic domains and hydrophilic regions swollen by water where most of charged repeat units and counterions are located. The size of hydrophobic regions decreases with increasing charge content. The microphase separation seems to be due to the effective interplay of two counteracting tendencies: hydrophobic association and electrostatic repulsion. When salt screening is added, the microphase separation is disappears.

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CURRENT STATE OF HIGH PRESSURE PHYSICS

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Introduction

High pressure physics as a branch of science was finally formed at beginning of the last century. Percy Williams Bridgman (1882-1961), Harvard professor and Nobel Prize winner, played a major role in development corresponding ideology, methods and experimental techniques. The term "high pressure physics" became widely used after Bridgman published a book under the same title in 1930. Experimental high-pressure physics deals with pressures ranging from one to few millions atmospheres (1 atmospheres = ~ 0.98 bar; 1 bar = 10^6 dyn / cm^2 = 10 Pascal (Pa)). Pressure variation in Nature is so much greater that hardly can be reproduced entirely in laboratory in near future. But it needs to indicate that the evolution the experimental technique made it possible now to model conditions existing in the center of the Earth. The history of development of high-pressure physics is not rich with remarkable discoveries like it is in a case of low temperature physics. One may characterize high-pressure physics as a modest workhorse of condensed matter physics. The citation of the 1946 P.W. Bridgman Nobel prize:

"for the invention of an apparatus to produce extremely high pressures and for the discoveries he made therewith in the field of high pressure physics" that didn't indicate any particular accomplishment just confirm this point.

However some important events and discoveries of the field must be pointed out. The discovery of the critical phenomena made by Thomas Andrews in 1961 and subsequent development of mean – field theory of phase transitions by van der Waals constitutes probably the major contribution of high pressure physics to science.

High-Pressure technique

Conventional (high volume) technique permits to achieve pressure up to about 200 kb and temperatures up to few thousands of K in volumes of order a few cm^3. However in recent years applications of the diamond anvil technique dominate in the most of all experimental efforts in the high pressure field. That extends the range of experimentally available pressures up to 2-3 Mbar but in volumes of a small fraction of mm^3. One of the important points that should be known to the general physics crowd is pressure measurement, which includes problems of pressure sensors and pressure calibration.

The most common pressure sensor for the diamond anvil setup is a ruby chip whose luminescence line is sensitive to pressure. But all the current calibrations of the luminescence line shift versus pressure suffer great uncertainties. Another point is that the straightforward way of squeezing a sample alone between anvils is a bad practice since uncontrolled non-hydrostatic stresses arise. A better way is to use a pressure medium, which stay nearly hydrostatic over significant range of pressure.

Equation of States and Phase transitions

Equation of states and occurrence of phase transitions are the most desirable information about properties of a substance at high pressures. In the past that information was available only on application of special technique, which includes using various kind of piezometers – often complicated unique devices. Nowadays the information on EOS and phase transitions of crystalline substances is routinely obtained by X-ray technique in diamond anvil cells. But gases, liquids and amorphous substances still require the old fashioned approach.

General character of behavior of substances at high pressure is illustrated in Fig. The only restriction for the form of the P-V compression isotherm consists in requirement of positive value of compressibility. In the opposite case a system becomes unstable. Virtually that kind of instability leads to phase transitions though it's some sort of a hidden feature and cannot be observed.

Equations of states are often of great practical interest like for instances the EOS of plutonium.

On the other hand since time of Wigner and Seitz for the first time calculated the cohesion energy of sodium precise experimental data on EOS of different substances serve a touchstone for various kind of theoretical approach to condensed matter physics.

Because of different nature of interaction in materials it was realized long ago that a universal EOS equally applicable to different classes of condensed substances doesn't exist. Though in macroscopic approach when using quantities: V, K, K', etc. one can get an equation that may be used for presentations of experimental data of materials of different nature in the wide range of pressures. I mean here in the first turn Birch – Murnaghan, Vinet and similar equations.

Modern microscopic approach to equation of states at T=0 is generally quite successful though may fail at describing some subtleties.

Phase transitions in solids at high pressures are so numerous that is impossible even briefly review this subject here. I will mention only some extraordinary examples. One of them is an isostructural phase transition in cerium observed by P. Bridgman. Discovery of the first order phase transitions in liquids is a result of recent development. Phase transitions in silica one of the major constituent of the Earth play important role in evolution of the Earth interior.

Miscellaneous

1. Quest for metallic hydrogen.

Since the paper of Neil Ashcroft, published in 1968, many attempts has been made to create the metallic hydrogen but so far despite all the claims nobody succeeded. Some new results of the effort are reviewed.

2. Metallization and superconductivity at super high pressure

Recently remarkable progress has been made in measuring resistivity at very high pressure. Due to this development a number of exiting results has been obtained.

3. Exotic crystalline structures

There was a general belief that at high pressure all substances acquire highly symmetric and close packed structures. This belief was destroyed by the recent discoveries.

4. Quantum phase transitions

Quantum phase transitions that occur as a result of quantum fluctuations at T=0 are intensively studied in recent years. The critical quantum fluctuations are believed to have special properties that provide strong glue for electron pairing.

FLNP JINR CONTRIBUTION TO THE EUROPEAN PROGRAMME «ATMOSPHERIC HEAVY METAL DEPOSITION»

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Air pollution by toxic heavy metals is of great concern in industrialized countries. A comprehensive survey of their emission into the atmosphere shows their negative influences on the environment and human health. In many European countries, increased efforts to establish heavy metal monitoring have lead to the international programme «Atmospheric Heavy Metal Deposition in Europe: - Estimations Based on Moss Analysis» [1]. Its objectives are to characterize qualitatively and quantitatively the regional atmospheric deposition pattern of heavy metals in Europe, to indicate the location of important heavy metal pollution sources and to allow retrospective comparison with similar studies repeated every 5 years. Concentrations of heavy metals in moss are closely correlated to atmospheric deposition and conversion to absolute deposition rates by calibration against the bulk precipitation data is rather straightforward [2].

Since 1995 Department of NAA FLNP JINR is involved in this programme reporting results to the European Atlas from moss survey 1995/1996 [3] on the Eastern Carpatians of Romania [4]. In 2000 the project «Atmospheric deposition of heavy metals in some industrial areas of Russia, Poland, Romania, Czech Republic, Bulgaria and Slovakia studies by the moss biomonitoring technique and employing nuclear and related analytical techniques and GIS technology» (REGATA) was accepted by the JINR Theme Plan and supported by grants of Plenipotentiaries of Poland [5], Bulgaria [6], Czech Republic, Slovakia [7] and two IAEA grants – for South Urals [8, 9] and Romania [4, 10]. Pilot studies were carried out in Central Russia [11], Western Ukraine [12], Serbia and Bosnia [13] and in summer 2002 in Macedonia [14]. More than 2000 samples were analyzed in Dubna using epithermal neutron activation analysis (ENAA) and in December 2002 the results were reported to the United Nations Economic Commission for Europe, International Programme on Effects of Air Pollution (UNECE ICP) to be included in the European Atlas 2000/2001.

A combination of instrumental ENAA in Dubna and AAS (atomic absorption spectrometry carried out at Geological Institute of RAS, Moscow, for Russia and in participating member-states) provide data for concentrations of about 40 chemical elements (Al, **As**, Au, Ba, Br, Ca, **Cd**, Ce, Cl, Co, **Cr**, Cs, **Cu**, Dy, Eu, **Fe**, Hf, **Hg**, I, In, La, Lu, Mg, Mn, Na, Nd, **Ni**, **Pb**, Rb, Sb, Sc, Se, Sm, Ta, Tb, Th, **V**, W, Yb, **Zn**) that substantially exceeds the requested number of elements (marked as bold) published by the European Atlas. Not all the above trace elements are strictly relevant as air pollutants, but they come from the multi-elemental analyses with insignificant extra cost, and most of them can be used as air-mass tracers. Applying multivariate statistical analysis to the data sets obtained it is possible to reveal the character and the origin of pollution sources within the area under investigation, as well as those sources affecting this area through long-range atmospheric transport.

Due to our contacts with the Department of System Analysis of Dubna University of Nature, Society and Man **GIS** (geographical information system) technology for the purposes of environmental monitoring is widely used for interpretation of the distribution of heavy metals over examined territories.

Department of NAA FLNP serves the basis for educating and training young specialists from many countries in nuclear analytical technique used for environmental studies in the framework of current international projects.

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HIGH-TEMPERATURE SUPERCONDUCTIVITY: UPS AND DOWNS

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After 16 years after the discovery of high-temperature superconductivity in 1996 by J. Bednorz and A. Müller in copper-oxide compounds, we still do not understand the mechanism of superconducting pairing. At present two main scenario survive: electron-phonon and magnetic pairing. The electron-phonon pairing was strongly supported in 2001 by "discovery" of field-induced superconductivity at 117 K in hole-doped fullerides intercalated with $CHBr_3$ which later appeared to be a false statement. Now we have the highest $T_C = 40$ K in the well established electron-phonon superconductor MgB_2, while high-temperature superconductivity with $T_C > 100$ K is observed only in copper-oxides. Therefore it is tempting to believe that the magnetic mechanism mediated by antiferromagnetic superexchange and spin-fluctuations is the genuine pairing mechanism in cuprates. A theory of high-temperature superconductivity caused by strong electron correlations developed by the author and coworkers will be presented.

JAHN-TELLER EFFECT AND THE ORIGIN OF FEROMAGNETISM IN THE MOLECULAR MAGNET TDAE-C_{60}

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Jahn-Teller effects have been proposed to play a key role in the extraordinary electronic properties of doped fullerenes such as high Tc superconductiviti and ferromagnetism. The fact that TDAE-C_{60} (where TDAE stands for tetrakis dimethylamino ethylene) has the highest transition temperature of all purely organic nonpolymeric ferromagnets has been specifically ascribed to a possible Jahn-Teller distortion and a resulting redistribution of the unpaired electronic spin density into a beltlikeform. No experimental observation of this effect has been, however, reported so far. Here we report the observation of a huge increase in the width of the ^{13}C NMR spectra of TDAE-C_{60} in the middle of the ferromagnetic phase at 10 K. This is due to a Jahn-Teller distortion of the C_{60}^- ions which becomes visible in view of the resulting changes in the Fermi contact electron $-^{13}C$ NMR shifts. The shape of the ^{13}C spectra allows for a direct determination of the beltlike redistribution of the unpaired electron spin density on the C_{60}^- ions, which is responsible for the relatively high ferromagnetic transition temperature in this purely organic system.

INELASTIC AND ELASTIC NEUTRON SCATTERING IN Cu_2Se

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IRRADIATING COMPLEX AT BIGR REACTOR AIMED AT SIMULATING ACCIDENTS OF RIA TYPE

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In connection with the access of Russia power engineering to foreign markets it is necessary today to increase competitiveness of domestic nuclear power plants (NPP). For this purpose there should be well-grounded the safety of reactors and performed licensing of existing and promising fuel what is impossible without experimental investigations of nuclear fuel characteristics.

Moreover, one of significant aspects consists in determining power thresholds of fuel elements failure with fresh and burnt out fuel under reactivity accident conditions and creation of database on fuel behavior under different irradiation modes and coolant states. Until recently the experimental base for such investigations performance has been absent in Russia.

Nowadays there is created at BIGR fast pulse reactor an irradiating complex aimed at simulating accidents of RIA type (Reactivity Initiated Accident) for fuel elements of different reactors containing both fresh and burnt out fuel. The investigated fuel elements are located in reflector-moderator block (RMB) with the characteristic dimensions of ~600mm placed right up to the side surface of the core. The operation outside the reactor core assists in increasing nuclear and radiation safety at carrying out experiments and makes it possible to vary within wide limits the configuration and composition of experimental assemblies.

In the paper there are described the procedures of calculation and experimental optimization of geometry and material composition of RMB itself and its components. The realized goal of such optimization consists in achieving the levels of energy input and, correspondingly, peak mid-radial enthalpy sufficient to reduce fuel element simulators with fresh fuel and refabricated fuel elements to failure.

There were produced two RMBs: on graphite base (RMB-1) and on beryllium base (RMB-2). Both versions are described.

For fuel elements with fresh fuel there are developed some tools to equip the investigated objects and corresponding channels to register processes and parameters characterizing fuel behavior and its response to pulse neutron effect. There was created proper software for measuring techniques and performed methodical substantiation of tests.

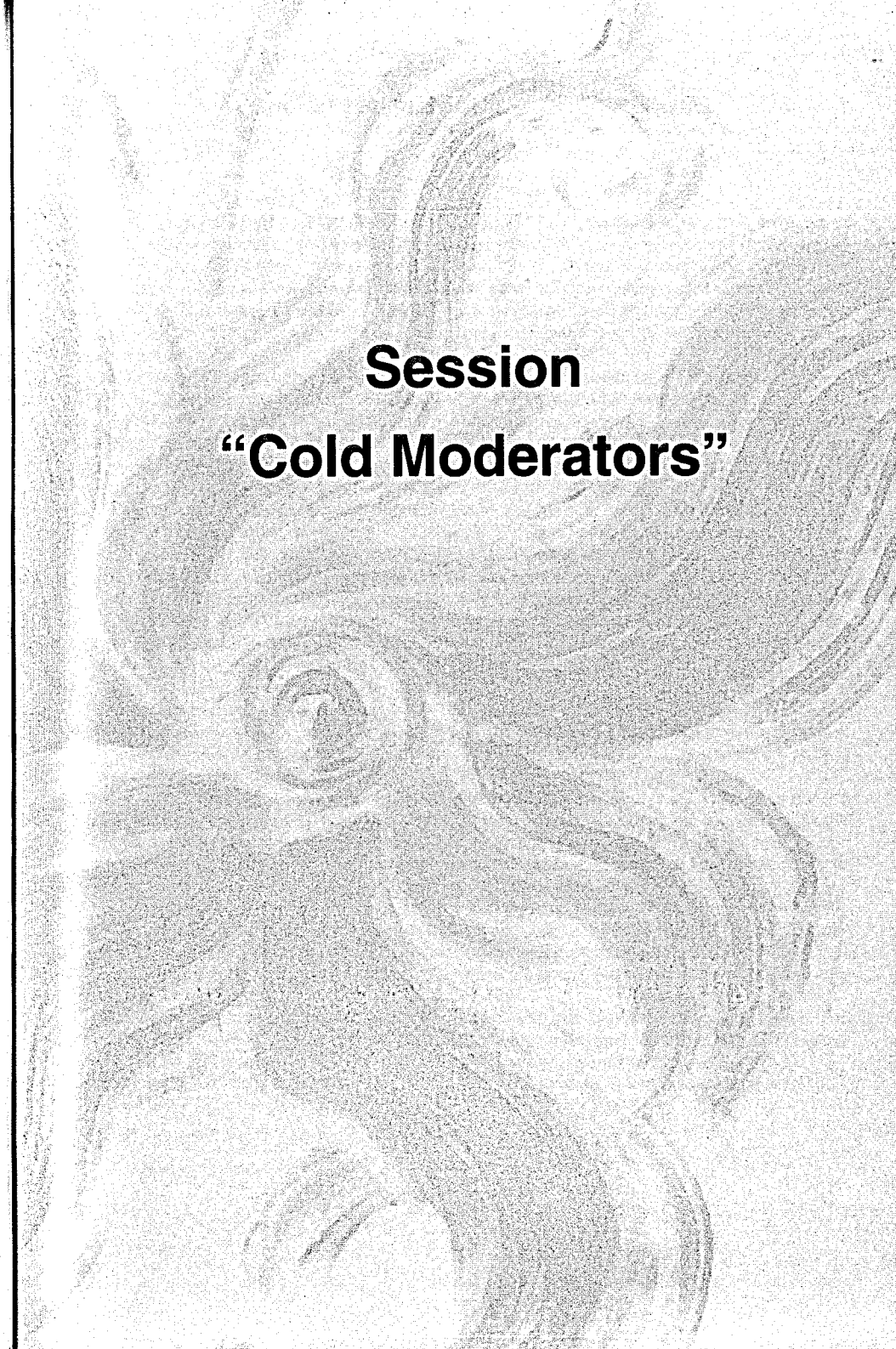
Refabricated fuel elements were produced and installed to tight ampoules in NIIAR where they were extracted after irradiation and then underwent investigations. To "close" the entire technological chain of tests there was developed and produced a transport package set (TPS) to transport re-fabricated fuel elements from NIIAR to BIGR and back. A license was achieved for the design of TPS and its itinerary.

Some series of fuel elements tests with fresh fuel and refabricated fuel elements (burnup – up to 60MWd/kg) were performed on the irradiating complex created.

There was obtained a considerable scope of information possessing high practical value in the field of creating database in verification codes on the calculation of fuel elements behavior under abnormal conditions.

Oral Presentations

Session
"Cold Moderators"



THE GIANT PULSES OF SLOW NEUTRONS IN BEAM-DUMPS OF PROTON. ACCELERFTORS FOR SUPERHIGH ENERGIES

Y.Y. Stavisski

The creation of the accelerator-storage complex LHC (CERN) opens the unexpected possibilities for research in the superhigh dense pulsed fluxes of low-energy neutrons (thermal, cold and ultracold). One of the wonders of nature is that, the circulation time of protons in big cycled accelerators is close to the lifetime of thermal neutrons in the hydrogenous moderators (H_2O, ZrH_2 and others). It is a base to produce the relative short thermal neutron pulses with giant peak flux density (up to ~ 10^{19} - 10^{20} neutr/cm^{2}s). By use other moderators possible produce the long pulses with more neutrons.

Yet Robert Wilson proposed to use the high energy proton accelerators (for tens and hundreds GeV) for "electronuclear breeding" (ENB). But it was a mistake - the most effective proton energy for ENB is about 1,2 GeV. The concurrence the direct proton ionization losses and the secondary ionization losses - through electron-photon showers caused by the π^0-s decay - give the broad maximum in the specific yield of neutrons near 1,2 GeV. The specific neutrons yield for lead at this maximum is about 24 neutr/proton GeV.

The high number protons, stored in big accelerators and his high energy give the possibilities, by using one-turn extraction, to produce a giant neutron pulses. For the low specified neutron yield (~ 2,5 neutr/proton GeV at 7 TeV), full yield is ~ 18000 neutrons per incident proton for 60 cm thick W-target. The main LHC mode provides the acceleration and storage of ~ 3.10^{14} protons with ~ 7 TeV and "cleaning" main ring every 10 hours by one-turn extraction into graphite beam dump. The calculations of V.G.Miroshnichenko (INR RAS) based on neutron yield for the thick tungsten target and the NeuMc code give the thermal neutrons peak flux in ZrH_2 moderator ~ $1.5.10^{19}$ neutr/cm^{2}s and thermal neutron pulse duration ~ 120 mcs.

For the neutron experiments my be used all intensity of LHC, without any harm interference with the classical particle program.

Such neutron source give the first possibility for the direct measurement of the neutron-neutron scattering length with high accuracy, that is significant for the fundamental hypothesis the nuclear forces charge independence.

The calculations of S.A.Novoselov (INR RAS) for the beam-dump LHC with W-target and ZrH_2-moderator show, that the neutron current from the vacuum cavity in the moderator through the neutron detector, caused by the n,n scattering in neutron gas, would be ~ 10^5 neutrons per one pulse. In one pulse may be received necessary statistical accuracy. It gives the hope for accuracy in n-n lengts experiment ~ 1 %.

It is appear the possibility for a research of new class multineutron nuclear reactions, when the nuclei captured a few neutrons before decay. Particularly, appear the possibility for the neutron-surplus transuraniums synthesis by the multineutron capture in heavy targets (f.e. ^{254}Cf, ^{257}Fm, ^{260}Md). It appears the possibility for investigations neutron interaction with radioactive nucleus too, including the originated by radiation capture during pulse.

The interesting research region my be connected with the neutron solid-state physics. For example - the neutron-photon scattering, particularly - experimental investigation the predicted amplification this process near phonon resonances in crystals (Agranovitch, Lalov, ISAN RF).

The considered heavy target in the beam-dump LHC will give the intensive neutrino fluxes too.

CONCEPTION OF COLD MODERATOR WITH SOLID AROMATIC HYDROCARBONS

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THE ESS MODERATOR CONCEPT AND INSTRUMENT LAYOUT OF THE SHORT PULSE AND LONG PULSE TARGET STATIONS

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The scientific application for ESS determines the selection of a reference suite of instruments for the both short pulse and long pulse target stations. The neutron beam spectral and pulse width properties are grouped into four sets of moderator properties serving the requests of the individual instruments.
At ESS this is fulfilled by a very versatile and flexible, large surface two-moderator concept for both short-pulse and long-pulse target stations. Novel features are the geometric combination and optimization of conventional liquid hydrogen and ambient water type moderator components. The results are:

- Four different viewing sides and large opening angles serving a total of up to 24 beam lines per target, from which two beam holes are used as horizontal moderator access and service lines.
- Individually adapted spectral and pulse width properties for each viewing fan to the request of the instrument suite.
- Broad spectral bandwidth moderators feeding neutrons into, for example, novel bi-spectral extraction beam lines.
- Easy to install option for virtually any other type of moderator and beam extraction system, e.g. advanced cold moderators of solid methane like spectra and ultimate intensity performance.

The geometry of the moderator assembly is presented and explained. General results of MC calculations on the expected neutronic performance and spectral properties are reported and the ESS facility layout and footprint of the instrument suite is explained.

NEUTRONIC STUDIES ON HIGH EFFICIENCY COLD NEUTRON MODERATOR FOR PULSED NEUTRON SOURCES

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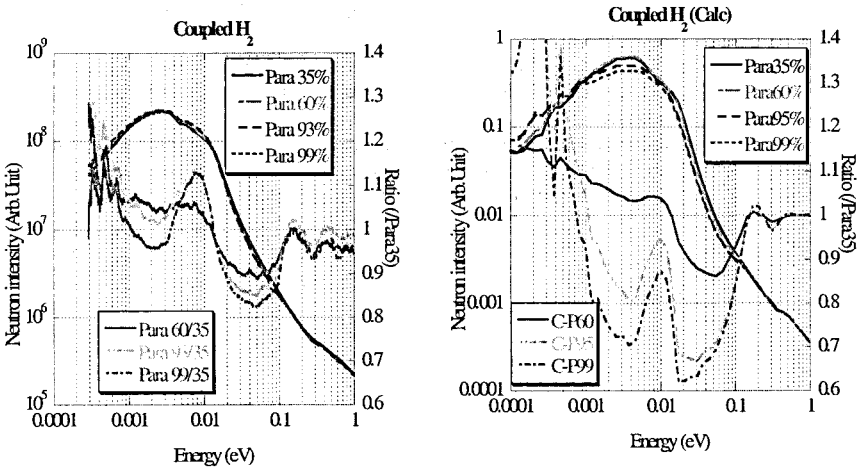
Cold neutrons are becoming more important for structure and dynamical analysis in the material science and bioscience, etc. Solid methane and liquid hydrogen are typical materials for the cold neutron moderator. Liquid hydrogen is a realistic candidate for a high power spallation neutron source since resistance to radiation damage is very high. We are studying the coupled moderators as high intensity moderator. We found that the coupled hydrogen moderator with 100% para gave higher intensity than that with normal para ratio by increasing the moderator thickness. Concerning to pulse shape (time distribution emitted from a moderator) para rich hydrogen moderator gives higher pulse peak intensity and faster decay of the pulse shape. These tendency have to be checked by experiments since the accuracy of the hydrogen cross section data have not been verified adequately. The figures shown below are comparison between experiment and calculation. Left figure is experimental results and right calculated ones. Intensity ratios are also shown. Para concentrations are indicated in the figures. There exist some differences in the energy spectra and also in the intensity ratio. However, the tendency in the calculation is similar to experiment. The intensity of a methane coupled moderator is almost the same as that of a hydrogen moderator with normal content, so a hydrogen moderator with 100% para may give higher intensity than the methane moderator

In this presentation we talk about recent progress of the neutronic studies on cold moderators.



INELASTIC NEUTRON SCATTERING AND SPECTRAL MEASUREMENTS OF ADVANCED COLD MODERATOR MEDIA

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Inelastic neutron scattering with emphasis on energetically low lying modes has been performed on four prospective advanced cold moderator materials. Employing the time-of-flight instruments SV29 and DNS at the Jülich FRJ-2 reactor, spectra have been obtained from synthetic methane clathrate, tetrahydrofurane (THF) clathrate, 1,3,5-trimethyl-benzene and light water ice at several temperatures between 2 K and 70 K. Clearly separated excitations at energy transfers of ±1 meV, +2 meV and +3 meV have been observed with synthetic methane clathrate. In hexagonal ice at T = 2 K up to now unreported low lying energy levels were found at energy transfers of 1.8 meV and 2.8 meV. An additional line at about 10 meV could be detected in the THF clathrate, which is most likely due to the embedded THF molecule. 1,3,5-trimethyl-benzene, synthetic methane clathrate and water ice, all at T = 20 K, have been tested as moderators at the Jülich spallation mock-up JESSICA. The expected gain in neutron leakage flux as compared to conventional liquid hydrogen moderators has been observed for methane clathrate and 1,3,5-trimethyl-benzene at neutron energies around 2 meV.

NEUTRON SCATTERING CROSS SECTIONS OF CRYOGENIC MATERIALS: PRELIMINARY RESULTS FOR MESITYLENE

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The Synthetic Scattering Function (SSF) allows a simple description of the incoherent interaction of slow neutrons with hydrogeneous materials. Its original formulation, essentially aimed at describing molecular gases, has been extended to include the important case of molecular solids. In any case, the main advantages of the Synthetic Model reside in the analytical expressions that it produces for double-differential cross sections and energy-transfer kernels, which in turn permit the fast evaluation of neutron scattering and transport properties.

More recently, we have introduced the concept of a Synthetic Frequency Spectrum (SFS) to represent in a simple manner the density of states of a molecular solid [1,2]. Using this approximation together with the standard NJOY code, we were able to obtain very good agreement with available experimental results for solid Methane, and make reliable predictions for the cases of water ice and Methane Hydrate [3,4].

In this paper we present the experimental total cross section of liquid (room temperature) Mesitylene measured in our laboratory, together with calculations for liquid and solid Mesitylene using preliminary versions of our scattering kernels for this material, based on the SFS concept.

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Juelich, Germany (Sept.2002).
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Workshop on Long Wavelength Target Stations, ISIS, UK (Feb.2003)

INELASTIC NEUTRON SCATTERING ON SOLID SOLUTIONS OF METHYL DERIVATIVES OF BENZENE SELECTED AS PROMISING COLD MODERATOR MATERIALS

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The selected organic solvents of methyl derivatives of benzene: toluene (1-methylbenzene) – $CH_3C_6H_5$, *m*-xylene (1,3-dimethyl-benzene) – $(CH_3)_2C_6H_4$, mesitylene (1,3,5-trimethylbenzene) and pseudocumene (1,2,4- trimetylbenzene) – $(CH_3)_3C_6H_3$, chosen for the study, have relatively low melting points of 180K, 225K, 227K and 228K, respectively. The CH_3 groups in free molecules of toluene, *m*-xylene and mesitylene have very low internal barriers for rotation with regard to C-C bound. The rotational modes of methyl groups are mixed with the lattice modes in the solid state of toluene [1] and m-xylene [2]. Mesitylene was assumed to behave similarly, therefore, it has been proposed and used as a cold moderator at pulsed neutron sources [3,4]. However, our recent neutron scattering investigation of this compound indicated three crystallographic phases of solid mesitylene [5]. When cooled, liquid mesitylene freezes in some disordered phase II, and at 90K it transforms to the low temperature ordered phase III, with high barriers for methyl rotations. At heating, phase II transforms to the stable phase I, the vibrational spectra of which look similar to those of solid toluene and *m*-xylene. Solution 3:1 by volume of liquid mesitylene and *m*-xylene, stabilizes the disordered phase II in all temperature range of solid phase. Solutions 3:2 by volume of liquid mesitylene with pseudocumene or toluene form glassy states in all temperature range of solid. The vibrational spectra of these disordered and glassy states of solid mesitylene in solution with toluene, m-xylene or pseudocumene, suggest that these materials should be preferred to be used as moderators for cold neutron sources.

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RADIATION PROPERTIES OF PROSPECTIVE MODERATOR MATERIALS

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Session "Neutron Instrumentation and Methods"

ULTRA-HIGH RESOLUTION NEUTRON DIFFRACTION USING FOURIER CHOPPER TECHNIQUE

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TOF contribution to a relative diffraction peak width $\Delta t_0/t$, measured with a time-of-flight diffractometer, is proportional to the width of the neutron pulse, Δt_0, and inversely proportional to the total flight path, L. Thus, it can be reduced either by shortening the source pulse or by increasing the flight path. The already existing and currently designed TOF high-resolution diffractometers exploit both possibilities: for instance parameters of HRPD at ISIS ($L\approx100$ m) allow obtaining $\Delta t_0/t$ as small as 6×10^{-4} in a wide d-range. Any further advances require the flight path which seems to be too long from the practical point of view. An alternative way for obtaining of very or even ultra-high resolution in neutron diffraction is using of the fast Fourier chopper and correlation RTOF method for data acquisition. The only existing at pulsed neutron sources, Fourier diffractometer HRFD [1] (located at the IBR-2 reactor, Dubna) with L=21.12 m, permits the TOF contribution to the resolution function as low as $\sim3.5\cdot10^{-4}$ with the chopper rotation frequency ω=9000 rpm. Both simple calculations and test experiments [2] show that with ω=11000 rpm and $L\approx30$ m, $\Delta t_0/t$ can be as small as 2×10^{-4} for d=2 Å. To attain this level with conventional TOF technique, one would need a flight path of about 300 m. In the paper the experience of operating of the HRFD instrument is presented and some key features of a Fourier RTOF diffractometer with ultra-high resolution are discussed.

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THE STRAIN DIFFRACTOMETER EPSILON-MDS AT THE IBR-2

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The most possible and comprehensive understanding of the deformation processes especially under conditions of the upper earth's crust is a requirement for a reliable evaluation of basal properties and its prediction for monitoring in geoengineering. A new quality of results concerning these problems can be expected from the development and application of new, interdisciplinar investigation methods. Such an innovation is just recently under development in theory and experiment on the base of studies concerning intracrystalline relations between strain, texture and stress in rocks using diffraction methods. A strongly required feature of these concepts is interdisciplinary cooperation, e.g. between geoscientists, material scientists, mathematicians.

First successful diffraction experiments in Dubna (1997) promised that we can get new answers to the mutual dependence of stress and texture forming processes within the earth's crust. The concept is based on the fact, that only strain, microstrain and texture might be directly measured, but they all together reflect the same reason: the stress field in earth. Experiments will be carried out with rock samples differing in structure and composition and under different regimes of applied load. Also consequences of possible residual strain/stress can be studied. It is possible to observe deformation processes *in situ* and furthermore to observe the time dependent process of recovery of residual stress equilibriums after drop of applied load.

The experimental fundament of those investigations is the neutron time-of-flight diffractometer EPSILON, situated at beam line 7A of the IBR-2 at JINR Dubna. Due to a flight path of 102 m a good spectral resolution ($4 \cdot 10^{-3}$ at 2Å) was achieved, nevertheless further improvements of the instrument were required because of the special characteristics of geological materials, like coexisting phases in combination with low grade symmetry. The spatial resolution, i.e. the selection of the gauge volume, is done by diaphragms both for the incident and the diffracted beam. The small gauge volume irradiated thereby and the long flight path lead to non-satisfactory intensity of recorded scattered neutrons. The aim of the modernization of EPSILON was to overcome this drawback and was in fact a total renewal.

The modernised instrument EPSILON-MDS, which worked for the first time in summer 2001, is equipped with nine radial collimators. The collimators are positioned on a ring, whose axis is parallel to the incident neutron beam. The collimators are arranged within three blocks, consisting of three collimators each, so that they are fixed at angles of –21°, 0°, 21°, 69°, 90°, 111°, 159°, 180°, and 201°. Each collimator has 48 gadolinium oxide coated mylar foils with an angle distance of about 20' of arc to each other and therefore covers a range of nearly 16° for 2Θ. In the other direction a range of about 18° is covered. The collimators are grouped to a unit of 66°. The transparency of the collimators is about 90-95%.

The detectors used are common ^{3}He-counter tubes with a diameter of 10 mm and an active length of 125 mm. The detectors are fixed in a plane also parallel to the incident beam. A gain in intensity is achieved by using an increased 2Θ-range for diffracted neutrons. The detectors are capable to record neutrons in the range $82° \leq 2\Theta \leq 98°$. Using a new developed time focussing method (choose of a individual, depending on 2Θ, channel widths for each detector), the spectra of all detectors belonging to the same collimator, can be added up automatically.

A COMPARISON OF DIFFERENT METHODS FOR IMPROVING FLUX AND RESOLUTION ON TOF-SANS INSTRUMENTS

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Small angle neutrion scattering (SANS) is one of the most popular and oversubscribed techniques at every user facility for neutron scattering studies of condensed matter that offers it.. The limiting features in SANS experiment design and the applicability of a given instrument to a particular problem of scientific interest are the length of time required to make a measurement and the minimum momentum transfer Q that can be measured. In the traditional pinhole-camera geometry, these two constraints are inextricably linked, forcing tradeoffs. However, three methods have been developed for reducing this linkage and thus allowing higher throughput while retaining high resolution and a low minimum Q in instruments that are still conventional steady-state or time-of-flight SANS instruments: multiple confocal pinhole apertures, focusing lenses, and elliptical mirrors. Each of these options has its own advantages and drawbacks; here we compare and contrast them and discuss their suitability for use at instruments at different types of neutron sources.

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THE MODERNIZED SMALL-ANGLE NEUTRON SCATTERING SPECTROMETER YuMO

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In this work we present the latest results on the modernization of small-angle neutron scattering spectrometer YuMO located on beam 4 of IBR-2.

The analysis of qualitatively new condition of a spectrometer is carried out.

It is shown that as a result of modernization and development of a small-angle neutron scattering technique, the range of accessible vectors of scattering is expanded, and also the dynamic range and speed of accumulation of experimental data are doubled.

The reasons for modernization are specified and the changes made in the units of the spectrometer (detectors, the detector of a direct beam, collimators as well as electronics) are outlined.

A few examples are used to demonstrate the improvement of background conditions, expansion of a q-range and a dynamic range.

The expanded possibilities on management of the spectrometer are listed.

In this work we also provide the comparative analysis of key parameters of installation before and after modernization. The questions regarding further development of spectrometer are considered and illustrated with examples.

DIRECT STRUCTURE DETERMINATIONS FROM HRPT NEUTRON POWDER DIFFRACTION DATA

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The implementation of the newest methods of structure determinations from powder neutron diffraction data (HRPT at SINQ spallation neutron source), in combination with the additional measurements done by Laboratory and Synchrotron X-rays (MS-P station at SLS), have recently allowed the structural characterization of various new compounds. The examples discussed will cover: the high-temperature phase transition in the $(Y_{0.92}Er_{0.08})BO_3$ borate, crystal and magnetic structures of the new layered manganese oxides A_2GaMnO_{5+y} (A=Ca, Sr) with brownmillerite-related structures, the new mixed cobaltite phase $HoBaCo_4O_7$, and some others. The insights into the possible approaches for the direct magnetic structure determinations from neutron powder diffraction data will also be discussed.

VISUAL DIALOG BASED ANALYSIS OF NEUTRON DIFFRACTION SPECTRA

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The report describes the further development of the VMRIA program, which is intended to analyze the neutron scattering spectra, obtained from the LNP neutron sources, first of all, the High Resolution Fourier diffractometer (HRFD).

This development proceeds in two directions.

1. Improvement of the program inner structure dictated by the interaction with the user via visual interface, offered by the DELPHI object-oriented programming in the WindowsXX environment.

In particular, main algorithm groups are implemented as DELPHI classes.

2. Extension of algorithmical abilities for the analysis of experimental neutron data: block for Rietveld analysis of the magnetic diffraction scattering has been included; the development of methods for the joint analysis of diffraction data from both neutron and X-ray sources is being performed; the development of analysis methods for different types of neutron scattering has been carried out, etc.

The similar development characterizes also the DELPHI program VDOMUS, intended for the analysis of multidimensional neutron diffraction spectra.

SOFTWARE PACKAGE AS (AUTOMATION OF SPECTROMETRY) FOR VME- AND CAMAC-STANDARD SPECTROMETERS AT IBR-2

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An instrumental software package (package AS) that enables prompt realization of experiment automation systems has been developed. In the development there were employed the new methods of programming and building of automation systems together with novel net technologies. The package is designed for experiments in condensed matter and nuclear physics and is ready for commissioning.

It is suggested that programs to schedule and conduct experiments should be based on the parametric model of the spectrometer, the approach that will make it possible to write programs suitable for any FLNP spectrometer and experimental technique applied and to use any hardware interface for the introducing of the spectrometric data into the data acquisition system.

The article describes the possibilities provided to user in the field of scheduling and control of the experiment, data viewing, and control of the spectrometer parameters. There is realized the possibility of presenting the current spectrometer state, programs and the experimental data in the Internet in the form of dynamically formed protocols and graphs and, with a password, of the experiment control via the Internet. To use the means of the Internet on the side of the client, applied programs are not needed. The realizability and effectiveness of the suggestions formulated in [1] have been confirmed.

Using the software package AS some variants of applied systems for electronics in VME- and CAMAC standard were created for the DN-2 spectrometer. The programs offered to user are easy to apply. It suffices to know how to use two programs to carry out experiments in the automated mode. The possibility of preliminary experimental data procession simultaneously with data acquisition is provided. To serve the purpose, user's programs written in any language, in particular those developed in the MATLAB system, can be involved in the process of data transformation. For two variants (VME and CAMAC) the systems of data acquisition and preliminary processing are linked to the system of final mathematical procession [2].

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A SETUP WITH A MECHANICAL CHOPPER FOR MONOCHROMATIZATION OF NEUTRONS AND TRUNCATION OF A NEUTRON FLUX OF THE IBR-2

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A setup was created for the investigations of a resonance structure of the neutron total and partial cross-sections in the energy below E<10 keV. It consists of two mechanical choppers of neutrons of rotor type with an engine of a direct current, an electronic stabilization system of the rotor's rotation and a phasing of the opening moment of slits along a neutron beam with a neutron pulse, collimators and neutron detectors. The angle velocity of rotation of rotors changes from 0 to 6000 r/min and their synchronization with the neutron pulse is provided with an accuracy of 10 mcs at the minimum opening time of slits along a neutron beam of 20 mcs. This setup is lightly transported and can be placed at any neutron beam of the IBR-2 or another neutron sources. The measurements of basic characteristics of the spectrometer have been made. They agree with the calculated ones within the experimental errors.

NEUTRON SPIN-PRECESSION IN A MAGNETIC FIELD AND WAVE RESONATOR

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Neutron spin-precession in magnetic field (Larmor precession) is connected with difference of two spin state (spinor components) wave vectors. A three-layered structure, whose first and third layers have a higher neutron optical potential than that of the intermediate (second) layer (U_1, $U_3 > U_2$), is a wave resonator in which realizes a phase shift of the neutron wave reflected from it if the neutron energy in the direction perpendicular to the interface $E_\perp$ lies in the interval $U_2 < E_\perp < U_3$ [1]. A wave resonator, whose first layer is ferromagnetic and as a result, the optical potential of interaction (U_1^+, U_1^-) of the neutron satisfies the conditions $U_2 \geq U_1^-$ and $U_1^+ \geq U_3$, changes the phase difference of spinor components (precession phase of polarization vector) and it names by the resonance spin-precessor. Action of resonance spin-precessor is connected with difference of ways for spinor components in resonator. In given report the investigation of properties of resonance spin-precessor is carried out. The resonance spin-precessor, was prepared as magnetic structure Fe(h)/Si(1200Å)/Cu(1500Å)/glass and has been studied by method polarized neutron reflection. The magnitizing magnetic field 10 Oe was directed in plane of the structure. Two neutron polarization rotators placed ahead of and after the structure have surved for rotation of polarization vector in plane and of plane which is pependicular to magnetic field direction. From measurements the changes of frequency spin-precession in a magnetic field were detected at some resonance values of neutron wave vector. The frequency changes follow of changes the precession phase at reflection of neutrons from structure. Simultenuasly the polarization efficiency decreasing is observed at increasing of h in range 50÷200Å. It can be connected as with noncollinearcy of an external magnetic field to magnetic induction in first layer as and with thickness variance of second layer.

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CURRENT SHEET SPIN-PRECESSOR FOR A NEUTRON SPIN-ECHO SMALL-ANGLE SPECTROMETER

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Polymers and biological objects are characterized by the correlation length $l_c=10\div10^5$ Å. Neutron small-angle scattering spectrometer with the thermal neutron wavelength $\lambda=1.5\div10$ Å and position-sensitive detection of a scattered beam allows to measure l_c in the range $10\div10^3$ Å. For measurement l_c in the range $10^3\div10^5$ Å a neutron small-angle spin-echo spectrometer has been proposed [1]. In such spectrometer the precession phase of the neutron beam polarization in a magnetic field determines the scattering angle. In this paper the spin-precessor based on the linear wires combined in two current sheets has been investigated. The slit geometry with horizontal scattering plane and vertical beam cross section has been used. The current sheets of spin-precessor are placed between the magnet poles under the angle θ_0 to the neutron beam in scattering plane. Neutron investigations of the spin-precessor with the distance 0.6 m between the current sheets and in the magnetic field 10 Oe have been carried out on REMUR spectrometer at IBR-2 reactor for the neutron wavelength range 1.5÷9 Å. The derivative on the scattering angle θ of the precessor polarization efficiency $P(\theta,\lambda)$ at the neutron wavelength $\lambda=3.8$ Å is equal to $\delta P/\delta\theta=86.3$ rad^{-1} and 109.9 rad^{-1} for the precessor angle $\theta_0=45^0$ and 27^0 respectively. From the obtained values of $\delta P/\delta\theta$ it follows that it is possible to carry out small-angle scattering investigations with this spin-precessor in the range $l_c=10^2\div10^4$ Å.

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ELASTIC AND INELASTIC NEUTRON SCATTERING ON ULTRASONIC EXCITATIONS IN SOLIDS STUDIED BY DIFFRACTION, NSE AND TOTAL REFLECTION TECHNIQUES

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The neutron interactions with acoustic waves observed by different methods is discussed.

Diffraction. [1-3] The influence of bulk ultrasonic acoustic waves on X-ray and neutron diffraction in the single crystals has been the subject of many investigations. The effects of the AW on the total intensity of the diffracted beam have been studied in detail. High-frequency ultrasound induces transitions between the sheets of the dispersion surface of neutron and X-ray in the perfect single crystals. These transitions lead in perfect crystals to the strong increasing of the diffracted intensity I_h and other effects. In deformed crystals these transitions lead to the drastic *decrease* (by up 50-70%) in I_h for *small* AW amplitude. Some fine oscillations, different for perfect and deformed crystals, are observed by us using single (Riga) and double-crystal spectrometers (Dubna). However the direct observations of the neutron inelastic scattering on such facilities is impossible because the energy of the ultrasonic phonons is very small, e.g. $E_s=413$ neV at $f_s=100$ MHz AW frequency and the difference in scattering angle between the phonon satellites is small too (~ several angular seconds).

Neutron Spin Echo. [4] For the first time neutron inelastic scattering on bulk externally excited ultrasonic excitations in single crystals (silicon, PG, mice and Kbr) and vitreous quartz was observed by using neutron spin echo spectrometer IN11 (ILL, Grenoble). Our approach opens up the way for the systematic investigation of ultrasonic excitations in different perfect and mosaic single crystals, polycrystals, glasses, amorphous materials, liquid crystals and so on. It is important that high quality single crystals are not necessary for these experiments. The important information concerning space distribution of amplitude and coherence of ultrasonic field was find by this technique.

Reflectometry .[5] As it was shown by J.Felber et al. [6] the energy exchange less than 10 nev between ultrasonic phonons and neutrons may be measured by reflectometry but only for very cold neutrons ($\lambda_n=2.4$ nm). The regimes of total and Bragg reflection of polarized neutrons from a layered structure was investigated by us as a function of the amplitude and frequency of transverse and longitudinal ultrasonic waves excited in the nanostructures and glass mirrors for $\lambda_n=0.2$ - 1.0 nm on spectrometers PNS-1 (Dubna) and for $\lambda_n=0.466$ nm on V-6 (Berlin). The off-specular reflection of neutrons and the shifting of the nodes and antinodes of the neutron wave field are observed. The probabilities of neutron inelastic scattering was determined.

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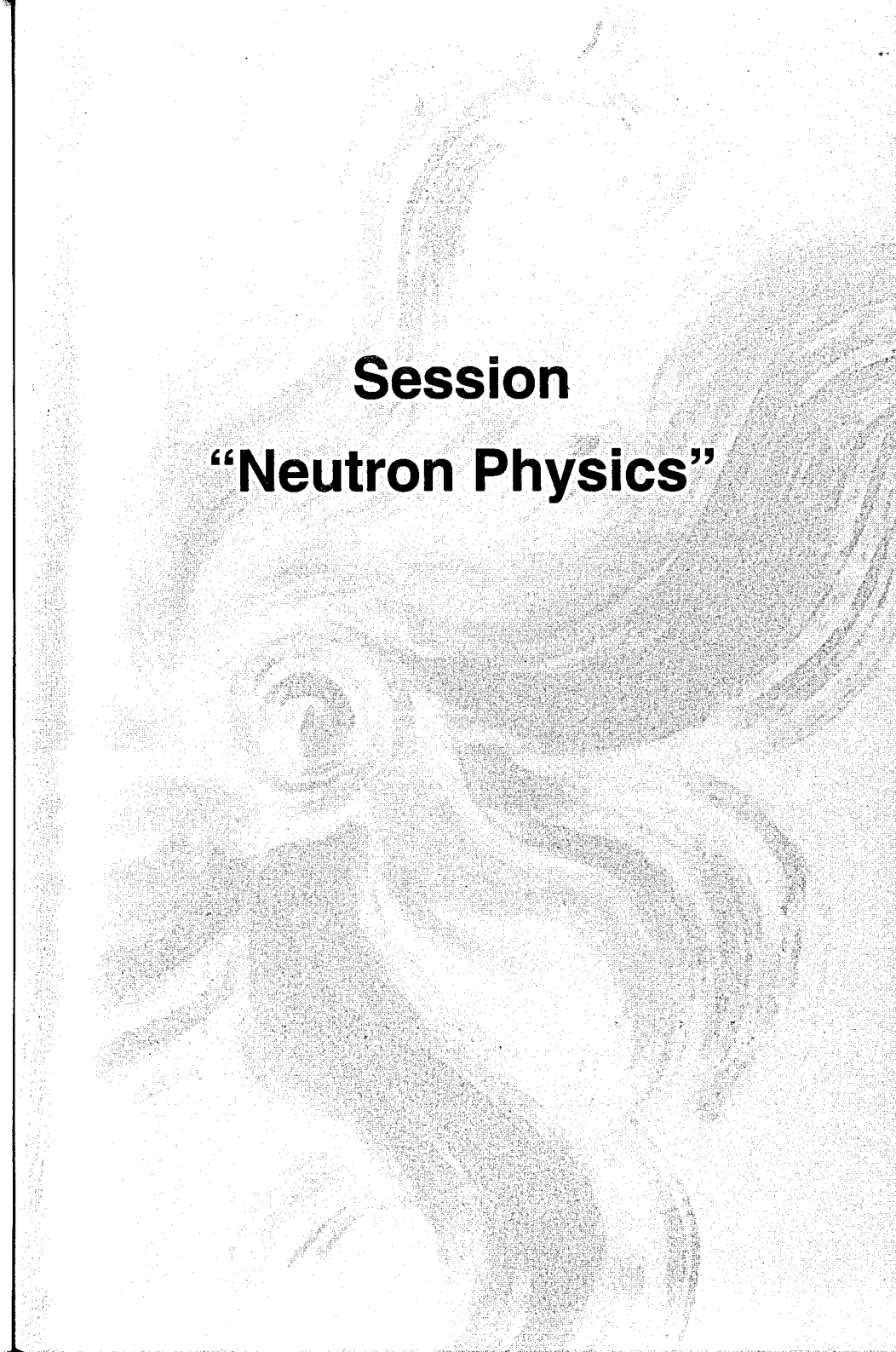

QUANTUM ASPECTS OF THE NEUTRON-INDUCED NUCLEAR FISSION

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FISSION PROCESS INVESTIGATIONS AT THE WHITE NEUTRON SOURCE GELINA

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At the European Commission, Joint Research Centre, Institute for Reference Materials and Measurements the **Geel Electron Linear Accelerator**, GELINA is used as a pulsed white neutron source for investigations in the field of neutron data for waste transmutation, accelerator driven systems, innovative reactor concepts, studying of the fission process, nuclear reaction mechanisms and standards.

In the present paper we will concentrate on recent neutron induced fission investigations of both ^{235}U and ^{239}Pu at resonance energies.

Up to about 200 eV all the resonances in the fission cross-section of those isotopes could be resolved. With a double Frisch gridded ionization chamber as fission fragment detector the mass and total kinetic energy (TKE) of the fission fragments could be determined. In case of ^{235}U fluctuations in the fission fragment properties have been observed as a function of the resonance energy. Although from a physical point of view even larger fluctuations should be visible in case of ^{239}Pu(n,f), no pronounced fluctuations in the mass yield and TKE distributions have been observed. The physics case is based on the fact that the only possible low energy spin states ($J^{\pi}=0^{+}$, 1^{+}) in case of ^{239}Pu belong to well-separated (about 1.25 MeV) transition state bands above the outer fission barrier. Hence, it was expected to observe differences in the fission fragment mass and TKE distributions between spin 0^{+} and 1^{+} resonances. However, no spin dependence could be distinguished.

Furthermore the experimental results have been interpreted within the multi-modality of the fission process [1]. To this end the Y(A, TKE) distributions have been unfolded taking into account three fission modes, two asymmetric and a symmetric one. The deduced branching ratios of the two asymmetric modes show similar fluctuations as the experimental TKE. Recently, a new theoretical approach has been put forward [2] in formulating a solution to the observed absence of the expected fluctuation of the fission fragment properties.

In case of ^{235}U also cross-section evaluations have been started taking into account the multi-modality of the fission process and based on experimental results obtained at IRMM. The results will be presented and discussed.

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MEASUREMENTS OF THE DOUBLE-DIFFERENTIAL NEUTRON SPECTRA IN FISSION OF U-235 AND Pu-239 INDUCED BY THERMAL AND RESONANCE ENERGY NEUTRONS

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Energy of the prompt fission neutrons have been measured in correlation with fission fragment energies and angles between fragment and neutron emission directions. Neutron beam was produced by the PNPI (Gatchina) WWR-M reactor. Fission fragment energies and emission angles with respect to the target plane were measured using a twin Frisch gridded ionization chamber. Neutron energy has been measured by means of time of flight method using 12 neutron detectors with pulse shape analysis for suppression of the gamma-quanta contribution. Gamma-quanta suppression coefficient was more than 10^4 at neutron energies range 0.5-15 MeV. Time resolution determined as a half-with of a gamma-fragment coincidence peak was 1.2 ns. A kinematical analysis of the obtained data has been made in the assumption of the isotropic emission of the neutrons in the center of mass system (c.m.s.) of fission fragment and dependence of the mean number of the emitted neutrons and the mean neutron energy has been obtained as a function of the fragment mass and energy. Measured characteristics of the fragment-fragment and fragment-neutron correlations have been preliminary analyzed and compared for fission induced by thermal and resonance energy neutrons.

SEARCH FOR HIGH ENERGY GAMMA-DECAY UP TO 200 MeV FROM THE SPONTANEOUS FISSION Cf-252

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ON THE MEASUREMENT OF THE FORWARD-BACKWARD EFFECT IN THE ^{35}CL(N,P)^{35}S REACTION

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We carried out the measurement and the evaluation of the forward-backward effect on the ^{35}Cl(n,p)^{35}S reaction with unpolarized, resonance neutrons up to 1keV incident neutron energy. In this energy range contribute two energy levels of the ^{36}Cl compound states E_S=-180 eV $J_S^{\pi}=2^+$ and EP=+398 eV, $J_S^{\pi}=2^-$. Using the model of mixing states with opposite parities of the compound nucleus we obtained the cross section, the differential cross section and the asymmetry coefficients. These coefficients are the forward - backward, the left - right and the parity non-conservation. In the thermal range of the neutron energy all the coefficients were evaluated to be of order of 10^{-4} and this is in a good agreement with our evaluation for the forward-backward effect and with evaluation from the literature for the other coefficients.

For the first time we have evaluated and measured the forward-backward effect in the energy region where this effect it is expected to have the maximum value. It is necessary to remind here that in this region the cross section it is of order of mb so the experiment is difficult due to the lack of statistics. Our theoretical evaluation of the maximal value is 0.30 and this value is in a direct dependence with the reduced amplitudes value form in the ingoing and outgoing channels of the neutrons. The maximal value for the forward-backward effect correlated with the value in the thermal region for the left – right; consequently, the parity non-conservation gives us the possibility to extract the matrix element of the weak interaction acting on the background of the nuclear reaction and to confirm the ^{35}Cl(n,p)^{35}S reaction contribution only from the spin channel with S=2.

The measurement of the forward-backward coefficient in the ^{35}Cl(n,p)^{35}S reaction was realized at IBR-30 facilities using a ionization chamber. The forward-backward coefficient values were determined for the averaged neutron energy range of 3.1, 195 and 398 eV, respectively, and these values are: $(5.3\pm7.6)\cdot10^{-3}$, $(1.68\pm0.50)\cdot10^{-1}$ and $-(7.4\pm3.6)\cdot10^{-3}$, respectively.

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RESEARCH OF CONTINUOS NUCLEAR-LASER INSTALLATIONS IN VNIIEF

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Investigations directed to using of nuclear energy for laser pumping have been carried out in VNIIEF since late sixties. The first successful experiments of obtaining of lasing in noble gas mixtures of atmospheric pressure excited by fission fragments in the neutron fields of research nuclear reactors were carried out in 1972. In other Russian and foreign (USA) institutions investigations of direct nuclear pumping of laser media were carried out later and since then they practically only repeated results obtained in VNIIEF and published.

Several experimental facilities for nuclear-pumped laser investigations were developed using pulse reactors existed in VNIIEF. Most of them were constructed on the base of VIR-2M and BIGR pulse reactors.

Two-channel laser installation LUNA-2M was developed just after the first successful experiments of obtaining of lasing in a gas. A lot of experiments were carried out on the VIR-2M/LUNA-2M facility to search and investigate nuclear-pumped laser media.

Lasing in visible and IR spectrum on more than 40 transitions of Xe, Kr, Ar, Ne, C, O, N, Cl atoms and Cd^+, Zn^+ ions has been observed and investigated in VNIIEF. Record parameters of nuclear-optical converters in a pulse mode were obtained (≈6 J/l,≈6 kW/l when efficiency of inserted energy was 2-2,5%).

During development of a continuous energy-intensive reactor-laser it is necessary to demonstrate the continuous mode of its operation and also to carry out its engineering and design debugging and to investigate characteristics of transverse gas pumping device.

The four-channel laser module LM-4 was developed and made to solve these problems. LM-4 installation consisted of four laser channels with 20□60 mm cross-section and active length of 1 m combined together with plate radiators into joined gas circuit with transverse gas pumping. Gas medium was excited by neutron flux from BIGR reactor. Pulse duration of BIGR reactor was about 1.5 s. Laser pulse duration was determined by reactor BIGR pulse duration. Continuous lasing in the nuclear-pumped lasers and effectiveness of transverse gas pumping were demonstrated for the first time in the world. Laser light power was near 100 W.

Now LM-4 is used to carry out experiments on addition of laser light from several channels and study of distribution of optical heterogeneity originating during excitation of a gas medium in order to form narrow directional diagram of the light beam.

Development of works in VNIIEF and achievement parameters suitable for practical application resulted in development of the reactor-laser conception as autonomous nuclear-physical facilities combining functions of the laser system and the nuclear reactor and making direct conversion of nuclear reaction energy into laser light /6/.

As a matter of fact a reactor-laser is a set of laser cells placed properly in the neutron moderator matrix. Number of laser cells can be from some hundreds to some thousands, the total weight of uranium amount can be varied from 5-7 kg up to 40-70 kg, typical linear dimensions of the installation is 2-5 m.

Basic energy, nuclear-physical, technical and operating parameters of different variants of reactor-lasers with laser power from 100 kW up to several megawatts were determined on the base of design-theoretical and experimental investigations, engineering and design debugging, experience of Russian reactor building, operation of research nuclear reactors and laser installation. These reactor-lasers could work in time modes from several seconds to continuous one. We considered reactor-lasers with heat accumulation in the core, when reactor's work duration was limited by permissible heating of the core (a heat capacity reactor-laser), and reactor-lasers with heat efflux outside the core i.e. not limited in power.

Advantage of reactor-lasers over other types of laser systems is determined by high specific and absolute power intensity being practically unattainable in other type of lasers, realization of effective transformation in a wide optical range, absence of intermediate steps of energy conversion, operation flexibility.

INVESTIGATIONS OF NUCLEAR-PUMPED LASERS USING VIR-2M PULSE REACTOR

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Practically all experimental investigations on searching for and study of nuclear-pumped lasers (NPLs) characteristics were carried out using pulse nuclear reactors [1,2], which differ in composition and design of reactor core, in pulse duration (5×10^{-5}-5×10^{-3} s) and neutron flux (10^{13}-10^{16} cm^{-2}), in volume and space configuration for sample irradiation, and pulse repetition rate as well. This circumstance may be explained by the fact that in steady-state nuclear reactors (IRT-2000 or VVR types) thermal neutron flux densities not exceed 10^{13} cm^{-2}, and such neutron flux level is insufficient for searching of new NPL active media and investigation of most known NPLs. In VNIIEF, for study of gas, liquid, and solid NPLs various types of pulse nuclear reactors were used: VIR-1M, VIR-2, VIR-2M, TIBR, BIR-2, BR-1, BIGR [1,2].

Water pulse reactor of VIR family [1-3] are the main facilities for investigations of NPL problems in VNIIEF during approximately 30 years. The first of them, VIR-1M reactor, was put into operation in 1964. By the way, pumping of laser medium by nuclear radiation was achieved for the first time in 1972 using VIR-2M reactor (He-Xe and He-Xe-N_2 mixtures excited by uranium fission fragments).

At present time, VIR-2M pulse reactor [1-3], which is forth modification of VIR-type water reactors, is widely used as neutron source for NPL investigations in VNIIEF. Reactor control system allows to put into practice two operating modes – pulse and steady-state. In pulse mode, the repeatable energy release in reactor core varies from 5 MJ to 60 MJ (1.7×10^{17}-2.0×10^{18} fissions). Difference between scheduled and virtual energy release not exceeds, as a rule, □1.5-2.0 MJ. Full width at half maximum amounts to 2.6 ms at energy release of 60 MJ.

The whole experimental facility consists of LUNA-2M (uranium layers, gas media), LUNA-2P (uranium layers, flowing gas media), and LYaN-2T (helium-3, gas media and metal vapors) laser setups, techniques for spectral-luminescent, laser, and optical investigations of various media, and techniques for studies of radiation-induced changes in optical materials and photodetectors, as well [4,5]. Each of laser setups consist of two laser cells which are identical with respect to design and irradiation conditions. The laser setups were placed in the lower hall of the building where reactor is located, on the remote-controlled trolleys.

To carry out investigation program on gas NPLs, about 3000 pulses of VIR-2 and VIR-2M reactors were produced from 1972 to 2003. As a result, the laser action in the visible and IR spectral regions on the 43 transitions of Xe, Kr, Ar, Ne, C, O, N, Cl atoms and Cd^+, Zn^+ ions was observed and investigated when atmospheric-pressure gas mixtures were excited by uranium fission fragments and the $^3He(n,p)^3H$ nuclear reaction products (see, for example, review articles [4,6]). Besides, some significant problems relating to investigations of optical and gas-dynamic characteristics of gas media were solved, and information needed for design of many-channel steady-state NPL [6] was obtained.

Now using experimental facility VIR-2M/LUNA-2M, investigations of xenon laser (which is most powerful among NPLs) at the wavelengths of 1.73, 2.03, and 2.65 μm are carried out. The main objective of these investigations is receiving of information on small-signal gain and saturation intensity using experimental data on energy laser parameters at various mirror reflectivities. As subject of inquiry, we are studied the He-Xe (□ = 1.73, 2.03, and 2.65 μm), Ar-Xe (□ = 1.73 and 2.03 μm), He-Ar-Xe (□ = 1.73, 2.03, and 2.65 μm), and

Ne-Ar-Xe (□ = 1.73 and 2.03 μm) mixtures. For these mixtures, it is possible to achieve lasing using only one from three laser lines when narrow-band cavity is used.

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MULTICHANNEL NUCLEAR-LASER DEVICES WITH QUASI-CONTINUOUS OPERATION AT BIGR REACTOR

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In the report there is briefly summarized an experience of LM-4/BIGR experimental facility maintenance from the viewpoint of development of multichannel laser devices with nuclear pumping of continuous operation |1-3|.

Within research carried out at experimental facilities LM-4 and LM-4M multichannel nuclear-laser devices were used with continuous operation that demonstrated validness of physical principles and engineering solutions taken as the basis of power reactor-lasers with continuous operation.

The laser radiation power from a single channel of LM-4 achieved 15-20W, and the energy of laser radiation from four channels of the facility was 100-150 J. At present these power parameters are the best for lasers with nuclear pumping.

During research performed at the modified laser module LM-4M there was demonstrated operation of a multichannel nuclear-laser device with continuous operation after durable (7 years) conservation of the unit; it was proved that it is possible to use consistent scheme of laser channel adding; there was also developed and applied an interferometric technique for monitoring of optical inhomogeneities and determination of energy resource in NPL pumping channels.

Advantages and disadvantages of laser modules under research are analyzed in the report. There is represented a construction of an eight-channel laser module with nuclear pumping being manufactured now for experiments at BIGR reactor. As the basis and an elementary cell for a new laser module a laser cell LM-4 is used.

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NEUTRON POLARIZABILITY

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In this report the problem of introducing the notion of neutron polarizability and the role of Prof. D.I. Blokhintsev in the development of this problem are discussed. The influence of neutron polarizability on neutron scattering by heavy nuclei is considered. The results of measuring electric neutron polarizability in the megaelectronvolt energy region and the energy region of less than 300 keV are correlated. The constant of van-der-Waals forces between neutron and heavy atom is estimated analytically. Some remarks are made in favor of the opinion that neutron polarizability was observed for the first time in neutron experiments, namely, in megaelectronvolt small angle neutron scattering, i.e. in 1957.

EXPERIMENTAL POSSIBILITIES TO INVESTIGATE THE NUCLEON – NUCLEON INTERACTION IN THE LOW ENERGY REGION

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CROSS-SECTION MODELING PROCEDURE FOR NUCLEAR REACTOR STEADY STATE AND TRANSIENT APPLICATIONS

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Over the past several years transients and accidents computer simulation and analysis for nuclear power plants has become increasingly important not only for licensing but also for increasing plant availability. Since the computer simulations have been greatly advanced they become capable of better estimating the parameters of under transient operation of nuclear reactor.

The purpose of this paper is to introduce a more accurate methodology of using neutron/thermal hydraulic analysis. The approach described in this paper is an original method of cross-section modeling. This work presents the methodologies for the development of the cross-section libraries which are used in neutron/thermal hydraulic calculations. This cross-sections have been prepared with help of the program WIMSD-5B (Winfrish Improve Multigroup Scheme version 5B). The automation of calculating and composing of cross-section library was made by using special tools that were prepared by the C++ compiler.

The obtained cross-sections are specific for reactor type WWER-440 Unit 1 Rivne Nuclear Power Plant, because of influence of such factor as composition of the core, variety of boron concentration during reactor company and total fuel cycle.

Composed cross-section library was successfully tested on the thermal hydraulic computer code RELAP5-3D. Comparison with data obtained using previous cross-section library illustrates higher grade of accuracy of the results of this work.

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VARIANTS OF APERIODIC PULSE REACTORS WITH FORCED PULSE PARAMETERS

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There were studied single (one-section) reactors with a core made of neptunium-gallium and uranium-molybdenum alloy as well as coupled two-section systems composed of a single pulse reactor and driven subcritical assembly made of uranium-molybdenum alloy or disperse uranium-graphite material. Neutron and kinetics characteristics of these systems were calculated. The information obtained together with data of earlier performed calculations allowed to make a conclusion on design aspects of reactor systems differing in a short radiation pulse at large volumes of core and cavity meant for samples location. It was demonstrated that the best pulse parameters belonged to the single pulse reactor made of neptunium-gallium alloy and related cascade system from this single leading reactor and driven subcritical assembly made of uranium-molybdenum material. Neutron fluence and γ-radiation dose in the region of samples location in the second system can be significantly amplified with the aid of converter of n-, γ-radiation.

The reactor with neptunium-gallium core possesses the axial cavity of 30 cm diameter. It is shown that in this reactor, in spite of a significant cavity volume, one can generate pulses with fast neutron fluence and a dose of γ- quanta ~ $1.3 * 10^{15}$ neutr./cm^2 and 1000 Gray, correspondingly, and the width at the half-height ~50 mcsec which is not achievable in reactors with uranium-molybdenum core. Due to threshold fissile material in this reactor there is no necessity for employing shields of neutron absorbing materials in the cavity and a possibility for revealing a dangerous auto-catalysis effect is decreasing. Besides, this reactor weakly responds to the action of surrounding objects and possesses a lowered pulse "tail".

The mentioned systems significantly surpass the acting pulse reactors in cavity volumes and combination of parameters of n-, γ- radiation pulse.

KINETICS OF CASCADE BOOSTERS IN THE ASPECT OF THEIR RAPIDITY AND SAFETY

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Results of Monte Carlo program calculations of simple spherically symmetrical systems simulating aperiodic booster are presented. The calculations were aimed at obvious demonstration of specific features of kinetics of cascade reactor systems and possibilities introduced by employment of the cascade effect principle in the aperiodic booster in the aspect of safety rise and improvement of time pulse parameters. There was also considered the goal of determining of moderator materials that are most promising from the point of view of booster parameters optimization. It was shown that at equal total numbers of fissions the neutron pulses in cascade booster, as compared to the one-section booster, were generated under conditions of a significantly deeper subcriticality and possessed a many-fold less duration. The highest pulse parameters were obtained in cascade boosters with neutron moderators made of tungsten, lead and molybdenum.

The assemblies cascade effect degree is rising as the moderator layer thickness is increasing. However, at large moderator thickness there reveals a significant effect of the parasitic capture of neutrons in the moderator leading to suppression of coupling factor k_{21} and decrease of booster efficiency rise rate. This condition mostly affects the system with tungsten, due to a high level of radiation neutron capture in tungsten.

Tungsten of 10-15 cm thickness as a neutron moderator in cascade boosters apparently excels other materials. But at large thickness values it is no more optimal. At 20 cm moderator thickness the highest value of booster efficiency exponent is attained in the booster with lead (8), the largest gain in subcriticality deepness is achieved in the booster with molybdenum (8, 3).

The work was fulfilled under the framework of ISTC project #1932.

ANALYSIS OF THE MULTISTEP EMISSIONS OF PROTON SPECTRA ^{40}CA (γ, P) REACTION AT ENERGY ε_G=60 MEV

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Within the framework of a modified quantum theory a statistical multistep compound (MSC) and direct (MSD) processes [1, 2], we carry out the calculation of the energy and angular distribution spectra of protons emitted from high excitation nucleus ^{40}Ca (excitation energy ε_γ=60 MeV), to obtain a result of absorption of γ-quantum nucleus pairs with excitation initial 2p2h state (the quasideuteron absorption). The compute code needed to account the emission spectra of photoprotons conditioned by various non-equilibrium multistep emission mechanisms is developed.

When the total impulse is conserved in the equilibrium and non-equilibrium photoprotons emission processes [3], the asymmetric part of the angular distribution of photoprotons is caused by the multistep direct emission (kMSD, κ=1,2,3,4) and the symmetric angular distribution of photoprotons is caused by the multistep compound (MSC) and combined (KMSD→MSC) emission mechanisms.

After the physical corrections the numerical description of energetic and angular spectra corresponding to all energetic regions of photoproton emission [4] is received.

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STUDY OF THE NEUTRON FLUX AND ENERGY AMPLIFICATION IN MULTI-ZONE SUBCRITICAL SYSTEMS WITH STATIONARY AND PULSE NEUTRON SOURCES

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A model of neutron amplifier made of a spherical subcritical system of enriched uranium with a point-like neutron source, located in its center is studied for both stationary and pulse neutron sources. With the help of the Monte Carlo MCNP-4C code, the dependence of the neutron flux amplification factor and the energy amplification factor on uranium enrichment, on the energy of the source as well as on the effective multiplication factor of the system is calculated.

We show that an amplification of the neutron flux by one or two orders of magnitude and two-three orders in energy is possible. The neutron flux amplification factor varies negligibly within the interval of 20–40% enrichments, falling drastically at lower enrichments. Thus, the system with 20% enrichment can serve as a good amplifier for both neutron flux and energy. Calculations of the amplification in two-zone systems, with and without a reflector confirm, in general, the idea about the application of the internal booster with $k_\infty>1$. This model can be used as a prototype for an intense neutron source or as an autonomous energy device (reactor).

MEASUREMENT OF SUBCRITICALITY OF SANDWICH-TYPE URANIUM-GRAPHITE MULTIPLYING SYSTEM

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Specific features of reactor-laser cores are their significant dimensions and, as a rule, a module structure characterized by a high porosity and well-defined anisotropy of the leakage neutron field /1/. Thus, creation of a mathematical model of such reactors even in the part of critical mass parameters calculations is a rather complex task, and its adequacy should be verified by direct physics experiments.

In this connection at VNIIEF a deeply sub-critical stratified uranium-graphite multiplying system (MS) was experimentally studied, and experimental values k_{eff} were compared with calculation values obtained by Monte-Carlo method.

In order to evaluate k_{eff} there was used a technique based on solution of inverted equation of reactor kinetics in one-point approximation /2/. This technique was tested in practice /3/ during changing of the VIR-2M reactor core whose fuel is water solution of uranium-sulphate UO_2SO_4. Sub-criticality was determined by analyzing transient processes which imply relaxation of MS towards a new equilibrium state after the disturbing factor stops affect the system. Transient processes were formed by a method of source "jerk".

Sub-critical experiments were conducted in geometry that practically excludes spatial effects what allows employment of reactor kinetics one-point model.

In the course of subsequent assembling of MS there was tested a range of subcriticalities $0.6 \le k_{eff} \le 0.73$, obtained (within standard deviations) agreement with calculation, and thus, verified the mathematical model of determining of reactor critical mass parameters which are a basis for reactor-lasers.

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NEUTRON FOCUSING IN TIME AT THE UCN DIFFRACTION BY MOVING GRATING

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The focusing in time of ultracold neutrons may prove very useful in solving the problem of accumulating ultracold neutrons in a trap that are generated by a pulsed source [1,2]. As was discussed in ref [3] the resonance neutron-spin flip or diffraction at a phase grating moving across a beam may used to implement time-controlled changes in the neutron energy and to achieved the effect of focusing. We report here about the first experimental observation of the neutron time focusing using nonstationary action at the neutron wave. Periodical accelerations and deceleration of neutrons was achieved by phase modulation of neutron wave with variable modulation frequency. Phase grating with variable space period moving across the beam was used for such modulation. The achieved efficiency of the neutron focusing was about 17 %. The possible application of this effect is discussed.

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INVESTIGATION OF A RESONANCE STRUCTURE OF THE TOTAL AND PARTIAL NEUTRON CROSS - SECTIONS OF NB, MO AND PB IN THE ENERGY REGION 0.100-200 KEV

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The neutron total transmissions and self-indication functions for the natural Nb, Mo and Pb have been measured at the 1006 m and 500 m flight pathies of the IBR-30 by means of the batteries with the ^{3}He counters and multisectional detector of gamma-rays. The metallic disks of different thicknesses and 80 mm diameter of Nb, Mo and Pb have been used as samples-filters for measurements of transmission functions. The total group and partial cross - sections and their self-shielding factors have been obtained from the ones in the energy range 0.100 – 200 keV. The experimental uncertainties of group cross sections and their self-shielding factors are 2-10%.

Analogous values were calculated by the program GRUCON with the use of the ENDF/B-6.7, JENDL –3.2 and JEF-2.2 evaluated data libraries.

MEASUREMENT OF THE $^{17}O(n,a)^{14}C$, $^{21}Ne(n,a)^{18}O$, AND $^{36}Ar(n,a)^{33}S$ REACTION CROSS SECTION FOR THERMAL NEUTRONS

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The measurements were carried out on the neutron beam of the IBR-2 reactor of FLNP, JINR. In experiment, a specially designed plate ionization chamber with a grid was used. The neutron beam formed by collimators went through the sensitive volume of the chamber located between the cathode and the grid. The chamber was filled with Ar, Ne, CO2, and ^{3}He in different proportions. The gas mixture served in the same time the counting gas as well as the gaseous sample. The cathode and anode signals from the reaction products are registered by a multiparameter data acquisition system. The calibration $^{3}He(n,p)^{3}H$ reaction was used for normalization to determine .the reaction cross sections.

The received thermal cross sections for the $^{17}O(n,a)^{14}C$ and $^{36}Ar(n,a)^{33}S$ reactions (233±12) mb and (5.43±0.27) mb, respectively, are in good agreement with the values of other authors. The $^{21}Ne(n,a)^{18}O$ reaction cross section (0.18±0.09) mb is more than in three orders of magnitude lower than the upper limit estimation reported earlier.

ON THE TRANSFORMATION OF THE NEUTRON RESONANCE INTO THE GROUND STATE OF A NUCLEUS

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According to a number of the experimental and theoretical works, neutron resonance (compound state of a nucleus) has extremely complicated in the structure wave function. On the other hand, the low-lying levels are very simple in the structure. It is of interest to understand the process of this transformation in the excitation energy diapason from ≈5 to eq ≈10 MeV. Some details of this process were revealed in the study of the two-step γ-cascades between the neutron resonance and a group of low-lying levels of about 50 nuclei with ordinary Ge-detectors.

This simplest experimental method allowed one to overcome earlier unsurmountable difficulties in the study of nuclear properties by the γ--ray spectrum when the spacing between its excited levels is less than the resolution of the existing spectrometers. These technical difficulties are made worse by the necessity to take into account the dependence of a probability of one or several successive γ--quanta on the structure of levels connected by them. At present, the two-step γ--cascades were studied in 50 nuclei --- from ^{28}Al to ^{200}Hg.

The main steps of the process under consideration look like following:

(a) in the energy interval by several MeV below B_n, the main part of the excited levels is, probably, presented by many-quasiparticle states or states whose phonon component cannot seriously affected nuclear properties;

(b) at the excitation energy $1\text{-}2<E_{ex}<3\text{-}4$ MeV for odd and even-even nuclei, respectively, level density and probability of γ--transitions between them are determined by the excitations of phonon type.

These conclusions (at the level of the working hypothesis) were made on the basis of existing theoretical notions and the following experimental results:

(a) above E_{ex}≈3-4 MeV, the density of the intermediate levels of the two-step practically exponentially increases as increasing E_{ex};

(b)~in the excitation energy interval $1\text{-}2 < E_{ex} < 3\text{-}4$ MeV, level density has nearly constant svalue.

Auto-correlation analysis of the excitation spectra of intermediate levels of cascade in this energy interval revealed probable «equidistant» bands consisting from, at least, three members. Their equidistant periods are approximately proportional to the number of boson pairs of the unfilled nuclear shells.

Final conclusion about the application of this picture of the process under study can be done after the investigation of two-step cascades in many local resonances of different target-nuclei.

Session
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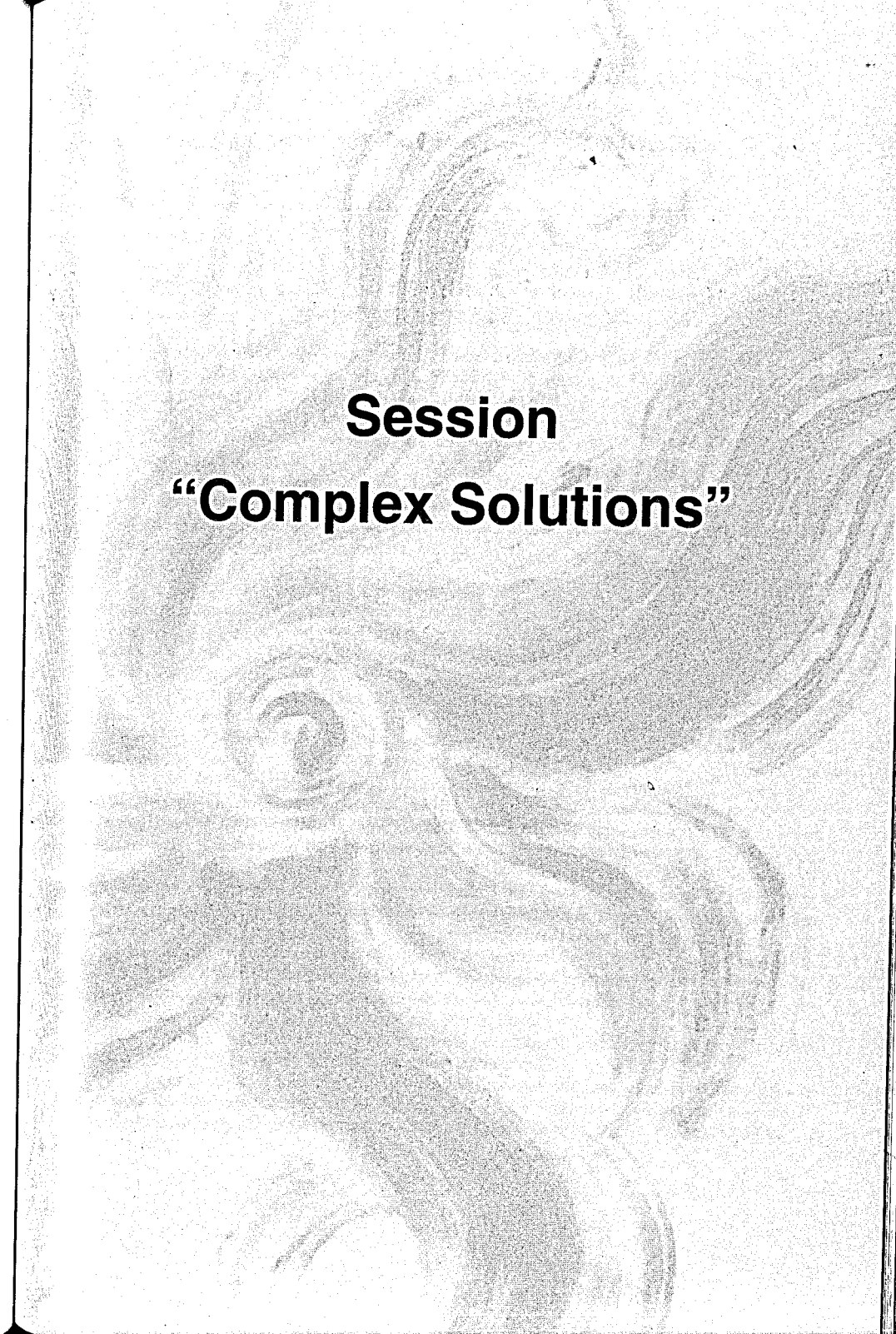

STRUCTURAL STUDIES OF FERROFLUIDS BY SMALL-ANGLE NEUTRON SCATTERING

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Magnetic fluids, also known as ferrofluids, are ultrastable colloidal suspensions of ferro or ferrimagnetic particles- e.g., magnetite (Fe3O4) - in various carrier liquids. The ultrafine magnetic particles, of 30-150A , "integrate" themselves in the structure of the carrier liquid by means of a surface active substance, which forms a protective "elastic" layer around each particle and together with Brownian motion, ensures the colloid stability even in strong nonuniform magnetic fields.

The neutron scattering methods have been largely used the last two decades for the determination of structural properties of magnetic liquids at microscopic level. There can be investigated the structure of the particle, the aggregation phenomena, the magnetic liquid dynamics, particle-surfactant interaction and the surfactant liquid-base interaction, magnetic dimension of the particles.

A highly suitable method for investigating magnetic fluids is the small-angle neutron scattering technique. The use of thermal neutrons makes it possible to study the structure of ferrofluids under a wide variety of experimental conditions. We present our investigations on ferrofluids performed for several years at different small-angle facilities including the YuMO time-of-fllight diffractometer at the IBR-2 pulsed reactor at the Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research (Dubna, Russia), SANS instrument at VVR-SM steady-state reactor at the Research Institute of Solid State Physics and Optics (Budapest, Hungary) and SANS setup at the SINQ spallation source at the Paul Scherrer Institute (Villigen, Switzerland).

The contrast variation method, applied in a small angle scattering (SANS) experiment, was used to simultaneously obtain information about molecular and magnetic structure of diluted magnetite/C6D6 ferrofluids. The effect of the colloidal particle concentration on the structure of the magnetite/C6D6 ferrofluid stabilized by oleic acid was investigated by SANS. It was shown that in the first case of the magnetite/oleic acid/benzene ferrofluid the thickness of the surfactant layer (monolayer of oleic acid around magnetite particles) changes significantly when changing the magnetite concentration. A significant decrease in the thickness of the surfactant layer with increase in the magnetite concentration is observed. This points to the fact that the interparticle interaction increasing with the concentration presses the surfactant tails in the layer closer against the magnetite surface. The magnetic scattering in the system was not taken into account, but the model curves fitted well to experimental ones, which points to a small effect of the magnetic scattering in the studied systems.

Further it was also studied in this systems the magnetic scattering by the analysis of the anisotropic SANS patterns from ferrofluids in a magnetic field.

In other case of the magnetite/ dodecylbenzenesulphonic acid/water ferrofluid the large interpenetration between sublayers of the double surfactant layer (dodecylbenzenesulphonic acid around magnetite particles) was detected which does not change much with the concentration.

DETERMINATION OF MULTILAMELLAR VESICLE PORTIONS IN EXTRUDED PHOSPHOLIPID DISPERSIONS BY SANS

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There is a wide variety of procedures for preparing vesicle dispersions. Independently of the method applied one obtains generally vesicles of different sizes with more or less broad size distribution (polydispersity) where the vesicles additionally contain different numbers of layers (multilamellarity). This is also true in the case of the extrusion method which is widely used for preparation of preferential unilamellar vesicles.

Recently Schmiedel et al. /1/ developed an analysis method which allows the determination of structural and hydration parameters from the part of the SANS resulting from the portion of the unilamellar vesicles. In order to extract this part from the total SANS measured the diffraction contribution resulting from multilamellar vesicles was modeled assuming that only bilamellar vesicles besides unilamellar vesicles are present in the dispersion.

In the present work it will be shown that quantitative parameters of the multilamellarity can be determined for the first time according to our best knowledge considering not only bilamellar vesicles but also vesicles with more layers in the frame of our approach. The agreement between the experimental data and the theoretical curves is simultaneously improved by this extension of our model. Obviously it reflects the physical reality better as the original approach.

Various POPC vesicle dispersions were prepared applying 5, 9 and 29 extrusions of a stock solution of 10 mg POPC in 1 ml D_2O through polycarbonate membranes with pores of 50, 100 and 200 nm. The SANS was measured in the q range of (0.009 – 0.36) A^{-1} using the small-angle neutron scattering diffractometer Yellow Submarine at the Budapest Research Reactor. The wide q range was realized by 3 overlapping q ranges determined by sample detector distances of 1.5 and 3.5 m and neutron wave lengths of 4 and 12 A.

Two SANS curves are represented in Fig. 1 and 2 as examples. The agreement between experimental data (filled circles) and theoretical calculation (line) is quite good in both cases. The two samples differ mostly in their multilamellarities; the first preparation contains 98 % unilamellar vesicles and only 2 % bilamellar vesicles and the second preparation 80 % unilamellar vesicles, 19 % bilamellar vesicles, and 1% trilamellar vesicles according to the analysis. The structural parameters of the POPC membranes in both preparations agree in the error limits as expected. The portion of multilamellar vesicles and the number of layers in the vesicles increase with growing sizes of the pores of the membranes used for the extrusion. The multilamellarity decreases with the number of extrusions.

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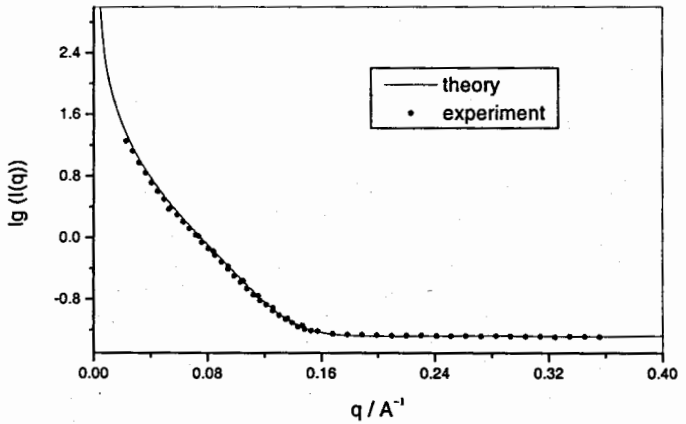

Figure 1 Data points (filled circles) and theoretical curve (line) of POPC vesicle dispersion prepared by 29 extrusions through polycarbonate membranes of 50 nm pore diameter

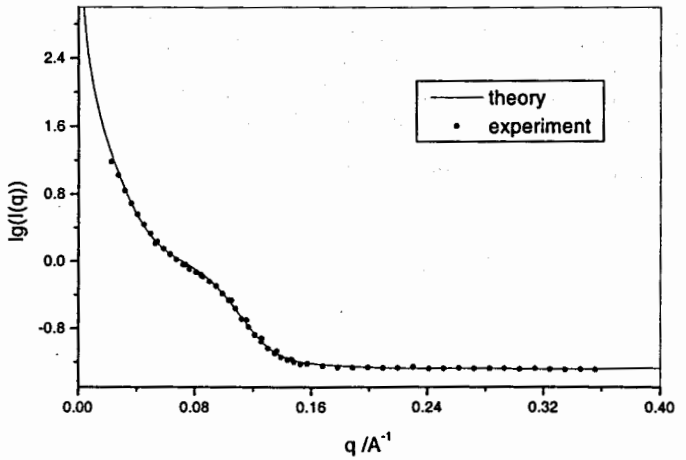

Figure 2 Data points (filed circles) and theoretical curve (line) of POPC vesicle dispersion prepared by 29 extrusions through polycarbonate membranes of 100 nm pore diameter

WHAT CAN WE LEAN ABOUT VESICLE STRUCTURE FROM SMALL-ANGLE NEUTRON SCATTERING EXPERIMENT?

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Methodologically, the membrane structure determination from small-angle neutron scattering (SANS) experiment on the unilamellar vesicles was developed via Kratky-Porod plot analyses based on the Guinier approximation [1]. Next step in the evaluation of membrane structure of vesicles was application of box model based on the strip-function approximation of the scattering length density across the membrane [2,3]. The disadvantage of both approaches was a necessity to apply other methods to determine vesicle shape. Model of separated form factors (SFF) was proposed to analyses the SANS curve from vesicles, which allows possibility to receive full information about vesicle shape, size, and membrane structure [4]. For the first time, without additional methods on the base of SFF model, the average radius and polydispersity of the vesicle population, thickness of the membrane bilayer, thickness of hydrophobic and hydrophilic parts of bilayer, and water distribution function were calculated [5]. The experimental results obtained at YuMO spectrometer in Dubna and SANS spectrometer at PSI, Switzerland are compared and discussed. The best conditions of SANS experiment at pulse neutron sources for the case of two scale structure are formulated.

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SOLUTIONS OF THE FULLERENES: EXPERIMENTAL STUDY AND MODELLING

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In the present paper the interaction of the fullerenes C_{60} and C_{70} with the solvents of aromatic family is discussed in detail. Experimental thermodynamic and structural data on solid solvates of C_{60} and C_{70} along with the data on solubility of the fullerenes are reviewed.

The unusual temeprarure dependence of solubility of C_{60} and C_{70} in aromatic solvents was explained by formation/incongruent melting of the solid solvates. Temperature of maximum solubility is a temperature of a first order phase transition in equilibrium solid phase (incongruent melting point).

The scaled particle theory (SPT) along with the polarizable continuum model (PCM) was used to describe the thermodynamics of solvation of the fullerenes C_{60} and C_{70}. According to SPT-PCM's resulting equation the solvation behavior of the fullerenes is determined mainly by the competition of the favorable dispersion interaction energy and the unfavorable energy of the cavity formation. The model was able to reproduce the general trends in solution behaviour of C_{60} in aromatic solvents and the transition to alkanes and water. According to the model C_{70} (compared to C_{60}) is more soluble in aromatic solvents but less soluble in water. The estimations were further extended to higher fullerenes, where the model predicted monotonous favourable changes of the solvation (not solution!) properties with the increase of the fullerene cage from C_{20} to C_{84}. The results obtained with SPT-PCM were compared with the ones of the widely used statistical approach based on the linear/non-linear correlations of the Gibbs free energy of solution with the certain solvent parameters.

Solid solvates of C_{60} and C_{70} were described with the help of the 6-12 Lennard-Jones atom-atom potentials (AAP). AAP were capable to reproduce both the thermodynamic properties and the crystal structures of the solvates. The model has also demonstrated its ability to predict the exothermicity of the solvate's formation.

Certain experimental evidence was found for the formation of the solid clathrate of hydrophobic C_{60} with water. This aggregate was precipitated from the water-fullerene dispersion prepared according to the method of Andrievsky[1]. Differential Scanning Calorimetry showed the presence of finely divided water, trapped inside the fullerene matrix. Surprizingly, the molar ratio of trapped water to C_{60} was the same in different samples studied. Possible models of the aggregate are discussed.

Similar effects were found with the SWNT[2], where solvents could occupy the interior gallery of the tubes and form "solvated tubes" stable due to non-covalent interactions.

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ON THE QUESTION OF CLUSTER STATE OF FULLERENES IN CARBON DISULFIDE. DATA OF SMALL-ANGLE NEUTRON SCATTERING

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The work concerns the problem of description of solubility behavior of fullerenes (C_{60}) in carbon disulfide (CS_2) with respect to temperature. Given dependence has a peak in the region of T=280K. A number of assumptions about the origin of this peak were made [1, 2] in recent years. In particular, it was explained [1] by a development of cluster state in the solution. The use [1] of the drop model to describe the cluster size distribution resulted in the mean aggregation number of about 13 at room temperature. The aim of the current work was to check out this point. To detect clusters the small-angle neutron scattering (SANS) was used. The experiments show that in C_{60}/CS_2 solutions small clusters of fullerenes are present, having the mean size of 4 molecules. The mean aggregation number does not depend on the temperature (15 ÷ 30°C) and concentration (4 ÷ 8 mg/ml). The obtained results cast doubt on the use of the drop model to describe the cluster structure in the solution. Results of previous SANS experiments with fullerenes in carbon disulfide are reviewed. The use of theory of nucleation for description of cluster state of fullerenes in carbon disulfide is discussed.

The work was carried out with the support of the Russian Ministry of Industry, Science and Technologies, state contracts №40.012.1.1.1148, №541-02.

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HYDRATED C_{60} FULLERENES - SUPRAMOLECULAR COMPLEXES OF CARBON AND WATER MOLECULES. STRUCTURE, PROPERTIES, POSSIBLE MECHANISMS OF THEIR UNIQUE BIOLOGICAL ACTIVITY

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In this report the main aspects determining physical and chemical properties of hydrated fullerenes will be discussed, and the basic mechanisms of their unusual biological activity will be examined.

1. What are aqueous molecular-colloidal solutions of hydrated fullerenes (**FWS**) and what are physical and chemical properties of hydrated fullerenes (**HyFn**) in the form of surprising, supramolecular, donor-acceptor complexes of $C_{60}@\{H_2O\}_n$! Model of hydrated C_{60} fullerenes strictures (in compliance with Molecular Dynamic Simulation) [1,2,3].

2. About some of the first data on the interaction of HyFn with nucleic acids, proteins and enzymes. About the experiments on their structures' stabilization in presence of HyFn via mutual stabilization of closed bounded water shells.

3. The facts about interactions of hydrophilic HyFn with living cells (with normal and malignant cells, as well with microbe cells and viruses etc.). HyFn don't influence on cell's viability functions and, at the same time, HyFn are able to prevent their membranes form destructive influences [4].

4. Surprising facts about antitumor and anti-atherosclerotic activity of water HyFn solutions. About biological efficacy of super small doses of HyFn [5].

5. About antioxidant properties of HyFn in vitro and in vivo systems. And possible mechanism of free radicals scavenge (or neutralization) by hydrated fullerenes (HyFn) that is determined by the water structures, which have been ordered by fullerene molecules.

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WATER-BASED FULLERENE COLLOIDAL SOLUTIONS BY MEANS OF SMALL-ANGLE NEUTRON SCATTERING TECHNIQUE

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The problem of fullerene solubility appeared after discovering the strong therapeutic activity of fullerenes in living organisms. Along with antioxidant properties fullerenes exhibit low ability of dissolving in polar solvents including water. A method of production of colloidal solutions was developed for medical purposes[1,2].

We've performed the small-angle neutron scattering (SANS) technique to investigate the solutions of C_{60} fullerenes in water with concentration of 0.002 ÷ 0.2 mM. The medical tests of the samples show the stability of colloids and possibility of medical use.

In the SANS experiments (Fig.1) we've obtained very high polydispersity of these colloids up to 500Å (what is confirmed by electron microscopy investigations[5]).The using of uniform spherical form-factors for the size distribution function is unable to describe experimental data. The method of contrast variation allowed us to determine a different from fullerenes component. Possibly it's responsible for the stabilization of the colloids. Some hypotheses including the formation of a specific hydration shell around the fullerenes, are discussed. There are attempts to draw an analogy to the system C_{60}/pyridine/water with a layer of pyridine around the fullerene aggregates as stabilizer[6,7].

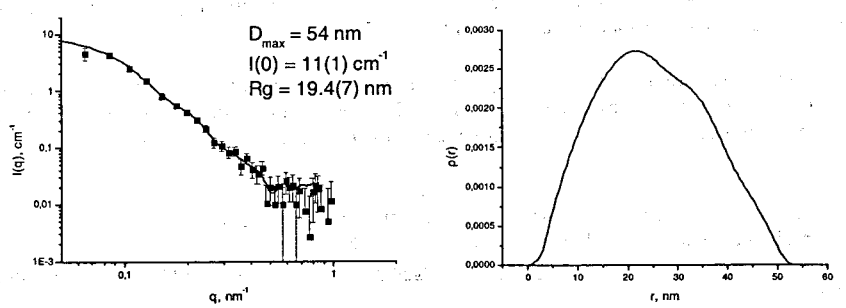

Fig.1. SANS curve (*a*) and the pare distance distribution function (*b*) for C_{60}FWS, c = 0.192 mM, T = 20°C.

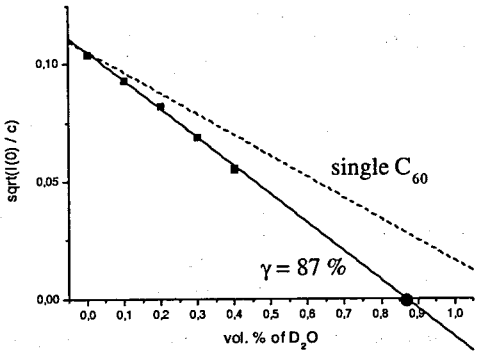

Fig. 2. Contrast variation for C_{60}FWS, c = 0.192 mM, T = 20°C; γ is the match point of the system corresponding to relative content of D_2O when the scattering from the aggregates disappears. Dashed line corresponds to behavior of the contrast as if fullerenes are single.

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TERNARY FULLERENE-PORPHYRINE-POLYMER COMPOUNDS: STRUCTURAL PECULIARITIES IN AQUEOUS SOLUTIONS STUDIED BY SANS

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Novel compounds tetraphenylporphyrine-C_{60}-poly(N-vynilpyrrolidone) of donor-acceptor type, synthesised in liquid and solid phase, have been investigated in aqueous solutions at ambient temperature by neutron small-angle scattering (SANS). The specific features of their hydration and structural organization in solutions as dependent on the enrichment of dry ternary systems with fullerene, C_F = 0-5 % wt., have been studied in SANS-experiments carried out in the range of momentum transfer $q=10^{-3}$-10^{1} nm^{-1}. The q-range covered the scales from monomer unit to mesoscopic fluctuations. The surroundings of the macromolecules were varied from light to heavy water to observe subtle details of hydration influenced by the isotopic composition of solvent. All the compounds have had the same amount of TPP (C_{TPP}=2 % wt.). Keeping a constant polymer concentration in solution (C_P=1 % wt.), we have started from double TPP-PVP-system. Increasing fullerene amount in the samples, we have observed the evolution of supramolecular structures from mass fractals (dimension D_M~2.3 without fullerene) to surface fractals (surface dimension D_S ~2.8, fullerene concentration C~2 % wt.). Meanwhile, the following doping induced opposite changes: the compounds, containing ~5%wt. of C_{60}, formed the mass fractals with dimension $D_M(C)$~2.9-2.8. Such behaviors of fullerene-containing molecular ensembles testify the cross-linking effect of fullerenes at low concentration (C_F<1%wt.). Above the critical concentration $C > C^*$ ~ 1 % wt. the scattering shows a nucleation in the system when a common polymer shell encapsulate a group of C_{60} molecules. Indeed, the scattering data manifests the drastic transformation of large molecular clusters (gyration radius R_G~200-500 nm) at fullerene content $C_F < C^*$~1% small entities (R_G~40-50 nm) at $C_F > C^*$. This resembles the formation of micelles in aqueous solutions of molecules having hydrophobic heads and hydrophilic tails. The overdoping with fullerene (C~5%wt.) leads to an anomaly in solubility. In other words, it improves the quality of the solvent that can be treated as a weakening of hydrogen bonds in water layers surrounding fullerenes. As we found, the observed structuring does not depend on the method of compound's preparation.

RECONSTRUCTION OF SHUNGITE FORMATION BASED ON STUDY OF COLLOIDAL SOLUTIONS OF FULLERENES AND NANOPARTICLES

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A novel branch of material science is appearing at the interface between molecular compounds and nanophase materials with promising technological applications. In this connection shungite (Sh) is a subject of considerable interest from both scientific and technological point of view. Complex and metastable structure of Sh has stymied its wide application and supplied a pursuit of special conditions of activation and stabilization of its nanosized units, mainly at Sh-liquid interface including catalytic behaviour, colloid and adsorption properties, cohesive energies, charge injection and transport in Sh-polymer composites.

Salient features of elemental carbon of Sh are connected with multi-shell units defining as globules, that were established by X-ray and electron diffraction, and scanning tunneling microscopy [1,2]. Since the methods describe different levels of structural organization, that corresponds to dimensions from a few up to hundred nanometers, further experiments (SAXS and AFM) were carried out to provide insight into reconstruction of Sh structural hierarchy reflecting the main steps of its formation. Structural organization of Sh suggested had some weak points that would be discussed in the paper.

Evidently, S with specific physical chemical properties was a product of geological processes in which water played an active role. Thus it would be challenging to look for the ways of reproducing of Sh structure from aqueous colloids in order to elucidate Sh structural organization.

Distribution of globules determined by AFM in the range from ten to hundred nanometers has shown that they exhibited a log-normal pattern similar to that for aggregation of drying.colloidal particles. The nanounits of Sh structure that could be removed into aqueous colloids from bulk Sh samples are the subject of the present paper.

Stable aqueous colloids of Sh and fullerenes were produced according to procedure described elsewhere in [3]. To study interaction in between nanoparticles TEM, AFM and SEM images were analyzed for both colloids. Morphological similarity of two colloids was discussed. Individual fullerenes could be hardly found in HRTEM images of fullerenes and Sh colloids. They are mainly organized into aggregates. Nanoparticles in the aggregates have no clear boundary between each other. The next level of aggregation was examined by AFM. The images of dried films of both colloids illustrated globular aggregates of hundred nanometers in size. SEM images showed flocculation of aggregates and formation of agglomerates (from several hundred nanometers to micrometers).

The work was supported by RFBR grant N03-03-32473.

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Session

"Biology and Polymers"

STRUCTURE AND DYNAMICS OF DENDRITIC MACROMOLECULES

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The recent state of structural and dynamical investigations for the macromolecules of dendritic (tree-like) spatial structure will be rewieved. The special attention will be payed to SANS measurements on dendritic macromolecules and new insight based on that results. Some possible practical applications of dendritic macromolecules will be discussed.

THE ENZYMES SUPERCOMLEXES. CLUSTERISATION OF MITOCHONDRIAL MEMBRANE PROTEINS

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The polyenzymatic systems can exist in two qualitative different states - dissociated and clustered. In present work the transition from dissociated form to cluster is considered on an example oxidative phosphorylation in mitochondria.

Besides that, feature of functioning of enzymes in structure of cluster, and also evolutionary aspect of a problem of clustering the proteins included in metabolic circuits is discussed.

INVESTIGATION OF POLYMERS BY NEUTRONS ON IBR-2

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Polymers as a biological samples are very common objects for investigation using small-angle neutron scattering. The structural information obtained via light and X-ray scattering is a mixture of contributions from individual polymer molecules and from groups of polymer molecules which is difficult to separate. The labeling methods were made possible due to the fact that the isotopes of atoms, particularly those of hydrogen, differ greatly in their abilities to scatter neutrons. SANS-technique gives the possibility to determine Gaussian chain and chain with excluded volume, swollen-branched chain; star and ring molecules; determine the persistence length and radius of gyration and hence, size of molecule. Some examples will be presented to illustrate many interesting results obtained so far using the YuMO spectrometer.

SMALL ANGLE NEUTRON SCATTERING STUDY OF THE INFLUENCE OF THE NATURE OF BOND BETWEEN HYDROPHILIC BACKBONE AND HYDROPHOBIC SIDE CHAINS ON THE STRUCTURE OF HYDROPHOBICALLY MODIFIED GELS

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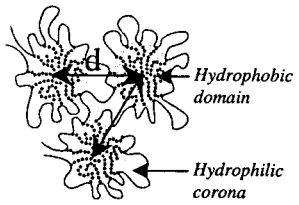
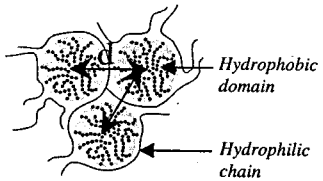
The structure of hydrophobically modified (HM) poly(acrylic acid) gels with different type of bond (covalent and ionic) between hydrophilic backbone and hydrophobic side chains was studied by SANS. Gel with covalent bond was prepared by radical copolymerization of acrylic acid with n-octylacrylate in the presence of cross-linker. Thus prepared gel contains immobile hydrophobic tails. Gel with ionic bond was prepared by complexation between carboxylic units of acrylic acid gel and n-octylamine in ethyl alcohol. Thus prepared gel contains mobile hydrophobic units. The hydrophobic tail content is the same in the both cases.

Neutron scattering curves of the both types of HM gels swollen by D_2O were compared at the same degree of swelling. There are peaks on the both curves. They characterize average distance between aggregates formed by n-alkyl groups. Specific length between aggregates was calculated from peak position for both cases. It equals to 50 Å and 31 Å for the gel with covalent and ionic links, respectively. The mean interaggregates distance for the gel with ionic links is correspond to the double length of hydrophobic unit. From these data the following structures of HM gels can be expected:

Gel with covalently bonded immobile tails



Gel with ionic bonded mobile tails



In addition, neutron scattering curves for the gel with ionic bond is characterized by a strong scattering at small angles, which indicates nonhomogeneously distribution of hydrophobic groups in the gel volume. Evidently these hydrophobic groups are concentrated in separate parts of the gel. Therefore, SANS data allowed us to reveal a quite different microstructure of the gels with fixed and migrating hydrophobic side groups.

This work was supported by Russian Foundation of Basic Research (grant No 02-03-33259) and by NWO grant.

NANOCHANNELS IN POLYMER MEMBRANES OBSERVED BY SAXS AND SANS AT STEADY AND PULSED NEUTRON SOURCES

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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. Small Angle Scattering (of X-rays and neutrons) 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]. Improvements in the PXY data treatment software [4] of SAS spectra allow to determine the channel diameter with its dispersion law, to demonstrate the existence of a wall thickness with a linearly varying density, and to assess the roughness [5].

PXY can also detect non cylindric shapes like single or double cones or spindles. SAXS measurements ha! ve been performed along SANS experiments on polyethyleneterephtalate and amorphous polycarbonate (aPC); the later exhibits channels with very small roughness. SAXS allows to make very precise characterisation of the nanochannels, while SANS provides an excellent determination of the conformation of the inserted material. SANS at steady and pulsed sources will be discussed.

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SELF-ASSEMBLED COPOLYMER-NANOPARTICLE THIN FILMS: STRUCTURAL ORDER AND MAGNETIC BEHAVIOR

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For the design of multicompositional materials with a spatially defined order of different components symmetric polystryrene-block-polybuthylmethacrylate P(Sd-b-BMA) lamellar thin films are used as structure-directing matrix for the nanoparticle arrangement. P(Sd-b-BMA) diblock-copolymer film spontaneously self-assembles upon annealing into a lamellar multilayer and order the PS-coated nanoparticles, incorporated into the polymer solution prior the annealing, in a periodic lamellar structure. Specular reflection and off-specular neutron scattering was applied to determine the distribution of magnetite Fe_3O_4 nanoparticles in symmetric P(Sd-b-BMA) films with a concentration of the nanoparticles from 0% to 7% of the volume fraction. From the experiments on neutron specular reflection and off-specular scattering we obtained information about the distribution of the nanoparticles within the lamellae and about the distortion of the lamellar order of the copolymer matrix [1].

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ANALYTICAL MODEL FOR DETERMINATION OF PARAMETERS OF HELICAL STRUCTURES IN SOLUTION BY SMALL ANGLE SCATTERING: INVESTIGATION OF BACTERIAL RECA STRUCTURES BY SANS

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Direct problem of small angle X-ray and neutron scattering on proteins and nucleoprotein filaments with helical structure in solution has been solved using a set of basic assumptions. The solution yielded analytical relationship between the scattering intensity and the main parameters of the helical structure. Based on the analytical solution for the direct problem and using an approximation of the first diffraction maximum, a minimization routine for the treatment of the reverse problem of small angle neutron scattering was implemented, which allowed us to obtain such structural parameters of protein filaments as mean diameter and helical pitch, as well as the radius of the protein monomer from experimental scattering curves.

Such a treatment of the experimental data allowed us to perform a comparative SANS study of the filament structures of RecA proteins from *E. coli* and *P. aeruginosa*, as well as of the thermosensitive mutant of the *E. coli* protein which had two amino acid substitutions in C-terminal domain (RecAEc2278-5). High degree of conservativity has been seen in the structure of the filaments formed by *E. coli* and *P. aeruginosa* enzymes in the presense of ATPγS ($RecA::Mg^{2+}::ATP\gamma S$), and in the structure of the presynaptic complex $RecA::Mg^{2+}::ATP\gamma S::ssDNA$ [1]. The parameters of the helical structure of the active presynaptic complexes of RecA proteins with ssDNA and non-hydrolyzable ATP analogues such as ATPγS and $ADP::AlF_4$ appeared to be very conservative for all three of the enzymes studied. Similar structural parameters were obtained for the active complexes formed by the proteins with an ATP analogue alone in high salt.

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EFFECT OF HIGH SALT ON THE FILAMENT STRUCTURE OF RECA PROTEINS FROM *E. coli* and *P. aeruginosa*: SANS STUDY

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RecA proteins play the key role in the processes of homologous recombination and post-replication repair in bacteria. Functional RecA enzymes are known to polymerise into helical filaments, which can in turn form nucleoprotein complexes by binding to nucleotides, such as ATP and ADP, and single stranded DNA (ssDNA). Formation of the tertiary presynaptic complex of the enzyme with both ATP and ssDNA is accompanied by significant changes in the structure of the protein filament [1]. Presynaptic complex of RecA enzyme exhibits ATPase activity and is capable of homologous pairing and strand exchange when double stranded DNA is present. The structure of such complexes appears to be relatively conservative for RecA proteins and its analogues [1, 2]. It has been shown earlier that in high salt conditions the ATPase activity can be induced in otherwise inactive complex of RecA protein with ATP alone [3], but the structural changes underlying this process remained unclear.

Two main parameters of RecA filament structure, the helical pitch and the mean diameter of the filament were evaluated by SANS on YuMO spectrometer (Dubna, Russia). Our data show that in the presence of 1.8 M NaCl and an ATP analogue the structure of RecA filament was similar to that of the active presynaptic complex of the enzyme. The increase in the helical pitch of the filament at different NaCl concentration could be described by hyperbolic function with half-point of about 0.5 M for *E. coli* RecA. The corresponding value for the *P. aeruginosa* enzyme was much smaller, about 0.15 M. The mean diameter of the helix decreased more gradually and could not be fitted to the same dependency of the salt concentration as seen for the helical pitch.

Our data suggest that in high salt RecA filament undergo similar conformational changes as those induced by binding of ssDNA during presynaptic complex formation. It appears that the changes in the helical pitch occur at lower NaCl concentrations than required for triggering enzyme's ATPase activity [3], and it can be supposed that the decrease in the filament diameter observed at higher salt concentrations is needed for the enzyme to assume its active conformation which is fairly conservative.

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SANS INVESTIGATION OF LIPID SYSTEMS AT THE YUMO SPECTROMETER IBR-2 REACTOR IN DUBNA

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As is known, a structural basis of cellular membranes is a lipid bilayer on which surface (or inside) there are proteins and other biologically important molecules. And this fact defines the importance of studying the complex systems on a basis of lipid systems. Neutron small-angle neutron scattering (SANS) has proven extremely useful in many applications (including biology and physical chemistry). SANS is a well established technique for measurement of membrane thickness in unilamellar bilayer vesicles and determination of bilayer's parameters of multicomponent lipid systems. In this report we briefly review the basic directions of biophysical research (including lipid systems) carried out at YUMO spectrometer.

SANS STUDY OF PHASE TRANSITIONS IN LIPID MEMBRANES AS FUNCTION OF LIPID/WATER CONTENT AND TEMPERATURE UNDER THE HIGH PRESSURE

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High pressure hydrostatic device was installed at the YuMO neutron small-angle scattering instrument for studies of biological and polymer solutions. The experiments were carried out for lipid/water dispersions. The thermotropic and barotropic phase transitions of DMPC/Water dispersions (multilamellar and unilamellar vesicles) at different contents from 1% to 17.5% wt/wt have been investigated by small-angle neutron scattering as a function of pressure and temperature up to 2 Kbar and 60°C, respectively. The results of experiments are discussed.

Session "High Pressure Physics and Earth Science"

HIGH PRESSURE INELASTIC NEUTRON SCATTERING STUDIES AT DN-12 SPECTROMETER OF IBR-2 REACTOR

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A technique for investigations of vibrational spectra of materials with large incoherent neutron scattering cross-section (typically, hydrogen-containing systems) by means of incoherent inelastic neutron scattering under high pressure up to 10 GPa using sapphire anvil [1] or tungsten carbide anvil [2] high pressure cells has been developed at DN-12 spectrometer [3] (IBR-2 high flux pulsed reactor, Dubna, Russia.

The results of resent experiments are reviewed. Vibrational spectra of ammonium halides NH_4X (X = F, Cl, Br, I) have been studied at pressures up to 8-10 GPa and room temperature [4, 5]. Ammonium libration mode and transverse optical mode frequencies as function of pressure were obtained.

An effect of high pressure on the hydrogen tunneling in α-Mn was studied at pressures up to 3 GPa in the temperature range 15 – 300 K [6].

An effect of high pressure on the inelastic neutron scattering spectra of AlH_3 has been studied.

An effect of isotope substitution on inelastic neutron scattering spectra of Ge is discussed.

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STUDIES OF PRESSURE-INDUCED STRUCTURAL AND MAGNETIC PHASE TRANSITIONS IN CRYSTALS AT DN-12 SPECTROMETER OF IBR-2 REACTOR

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The results of the recent studies of pressure-induced structural and magnetic phase transitions performed at DN-12 spectrometer (IBR-2 high flux pulsed reactor, Dubna) using sapphire anvil high pressure cell technique are reviewed.

A crystal and magnetic structure of manganites $La_{0.67}Ca_{0.33}MnO_3$, $Pr_{0.7}Ca_{0.3}Mn_{1-y}Fe_yO_3$ (y = 0, 0.1), $Pr_{0.8}Na_{0.2}MnO_3$ has been studied in the pressure range up to 4.5 GPa and temperature range 16 – 300 K. In $Pr_{0.7}Ca_{0.3}MnO_3$ and $Pr_{0.8}Na_{0.2}MnO_3$ a phase transition from pseudo-CE type antiferromagnetic (AFM) state to A-type AFM state was observed under high pressure. In $La_{0.67}Ca_{0.33}MnO_3$ and $Pr_{0.7}Ca_{0.3}Mn_{0.9}Fe_{0.1}O_3$ a phase transition from ferromagnetic (FM) state to A-type AFM state was observed under high pressure.

A crystal and magnetic structure of MnAs has been studied at high pressures up to 4 GPa in the temperature range 16 – 300 K. An appearance of a new magnetic phase with a complex magnetic structure having AFM and FM components was observed under high pressure.

A crystal structure of mercury chalcogenides $HgSe_{1-x}S_x$ and $HgTe_{1-x}S_x$ has been studied at high pressures up to 4 GPa. A pressure-induced structural phase transition from cubic zinc blende to hexagonal cinnabar phase was observed.

The work has been supported by the Russian Foundation for Basic Research, grant 03-02-16879 and Russian Ministry of Science, Industry and Technology, State contract № 40.012.1.1.1148 and grant of support of unique facilities of Russia.

A NEW NEUTRON DIFFRACTOMETER FOR HIGH-PRESSURE RESEARCH AT THE IBR-2 PULSED REACTOR

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At the IBR-2 pulsed reactor (FLNP, JINR, Dubna) a program of neutron diffraction studies of atomic and magnetic structures of crystals under high pressure is developing during about 10 years. As usual these studies are performed with DN-12 diffractometer, which has been built in the frame of collaboration between FLNP and "Kurchatov Institute". A studied sample is placed into high-pressure cell between single crystal sapphire (up to ~70 kbar) or diamond (up to ~200 kbar) anvils. The special detector system with high solid angle and precision construction of incident neutron beam path offer a possibility for measuring small (2 - 5 mm^3) samples in reasonable (several hours) time [1]. A substantial advantage of high-pressure cells with single crystal anvils is their small size, which is important for low temperature studies. As usual there is no problem to cool a cell down to 10 – 15 K.

Despite of evident progress the luminosity of neutron diffractometers for high-pressure research should be substantially improved. It is needed, for instance, for phase transition studies, when temperature or pressure scanning is obligatory. The only way of luminosity improvement is adaptation for high-pressure diffractometers of advanced detectors with large solid angle.

At FLNP a design work on new high-luminosity diffractometer for micro-samples studies under high-pressure was started recently. High luminosity will be achieved by using of many (up to eight) detector rings, each of that is formed by 16 helium counters. Another possible variant is development of specialized detector on the base of ZnS(Ag) plastic scintillators. The main problem, which should be resolved, is mutual adaptation of high-pressure cells and detector system providing a maximum solid angle. Another purpose of the work is a solution of questions connected with lowering of background, experiment automation and data processing.

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INFLUENCE OF HIGH PRESSURE ON CRYSTAL AND MAGNETIC STRUCTURES OF MANGANESE ANTIMONIDE BY NEUTRON DIFFRACTION DATE

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Neutron diffraction experiments have been performed on the manganese antimonide by the pulse reactor Frank Lab of Neutron Physics JINR. Influence of high pressure on crystal and magnetic structures have been investigation by neutron diffraction.

This compound crystallizes in tetragonal structure of Cu_2Sb type (C 38) of original block-layered character having high sensitivity of interatomic interactions to changing structure-size parameters (interatomic distances, bond angles, structural positions). Mn_2Sb is a ferrimagnet (T_C = 550 K). It is found that the type of crystal structure and magnetic orderings does not change up to P = 5.3 GPa at T = 300 K. Spin reorientation relative to crystallographic axes takes place at the $P \geq 2.8$ GPa. Lattice parameters *c* and *a* decrease when the pressure increases. The compressibility coefficient along *a*-axis is twice as much as that along *c*-axis. Thermobaric treatment of Mn_2Sb (P = 7 GPa, T = 1500 K) leads to polymorphous transformation from tetragonal to orthorhombic structure with a sharp change of magnetic state. Magnitometry data show zero resulting magnetic moment. Neutron diffraction patterns of high pressure Mn_2Sb phase indicate the presence of antiferromagnetic ordering in low temperature region ($T_N \cong 200$ K).

The results are discussed on the basis of model of interactions between crystal and magnetic subsystems in the materials.

LOCALISATION OF HYDROGEN AND DEUTERIUM IN B MANGANESE

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The solubility of hydrogen in α- and β-Mn under high hydrogen pressures reaches a few atomic percent [1]. No interstitial phases based on the α- and β-Mn type metal structure have been studied before. Our neutron diffraction investigation has shown [2] that H atoms in α-Mn occupy the 12*e* type interstitial positions arranged in small dumb-bells 0.68 Å long. The results of inelastic neutron scattering (INS) gave conclusive evidence of the low site symmetry of these positions and the tunneling effect. This paper presents results of a neutron diffraction study of the solid solutions of 10.8 at.% deuterium and of 9.6at.% hydrogen in β-Mn carried out with the D1B diffractometer at ILL in Grenoble and with the HRFD at LNPF in Dubna. It is shown that hydrogen or deuterium forms an unusual sublattice in the β-$MnH(D)_x$ high-pressure phase and occupies the (1/8, *y*, *y*+1/4) positions of the cubic space group $P4_132$ (No.213). The spectrum of optical vibrations in $MnH_{0.096}$ was also studied by INS at 5 K using the IN1 BeF spectrometer at ILL. The fundamental band of optical H vibrations is found to be split to two peaks in agreement with the H site symmetry.

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HIGH PRESSURE NEUTRON DIFFRACTION STUDIES OF THE UME_2GE_2

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Effects on high external pressure on the magnetic structure of $U(Pd_{1-x}Fe_x)_2Ge_2$ have been studied. The comparison between changes of crystall lattice parameters and interatomic distances showed that high external pressure induced more stronger changes in the crystal structure than „chemical pressure" by variation of Fe content or substitution Fe by Co and Ru. The interatomic distance U-Me at applied pressure up to 4.1 GPa changed almost in 9 times more, than at increasing of Fe doping level from 0 to 0.03. Possible explanations of the changes in the magnetic structure is discussed.

NEW APPROACH TO THE HIGH PRESSURE STUDY OF THE 3-D ELASTIC ANISOTROPY

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New high pressure system was designed for the study of elastic anisotropy of condensed matter under high confining pressure up to 700 MPa. Simultaneously could be measured dynamic and static parameters: a) dynamic parameters by ultrasonic sounding, b) static parameters by measuring of spherical sample deformation. The measurement is carried out on spherical samples diameter 50 ± 0.01 mm. Higher value of confining pressure was reached due to the new construction of sample positioning unit. The positioning unit is equipped with two Portecap step motors, which are located inside the vessel and make possible to rotate with the sphere and couple of piezoceramic transducers. Sample deformation is measured in the same direction as ultrasonic signal travel time. Only electric leads connects inner part of high pressure vessel with surrounding environment. Experimental set up enables: - simultaneous P-wave ultrasonic sounding, - measurement of current sample deformation at sounding points, - measurement of current value of confining pressure and – measurement of current stress media temperature. Air driven high pressure pump Haskel is used to produce high value of confining pressure up to 700 MPa. Ultrasonic signals are recorded by digital scope Agilent 54562 with sampling frequency 100 MHz. Control and measuring software was developed under Agilent VEE software environment working under MS Win 2000 operating system. Measuring set up was tested by measurement of monomineral spherical samples of quartz and corundum. Both of them have trigonal symmetry. The measurement showed that the P-wave velocity range of quartz was between 5.7 – 7.0 km/sec. and velocity range of corundum was between 9.7 – 10.9 km/sec. High pressure resistant LVDT transducers Mesing together with Intronix electronic unit were used to monitor sample deformation. Sample deformation is monitored with the accuracy of 0.1 micron. All test measurements proved the good accuracy of the whole measuring set up. This project was supported by Grant Agency of the Czech Republic No.: 205/01/1430.

APPLICATION OF NEUTRON DIFFRACTION TO STUDY OF ANISOTROPY AND TEXTURES OF ROCKS AS FACTORS OF "GENETIC MEMORY" FOR DEFORMATIONAL AND METAMORPHIC PROCESSES IN THE LITHOSPHERE OF THE EARTH

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The fundamental problem of geology and geophysics deals with the investigation of rock structure, formation and modification during evolution of Earth's lithosphere on different scale levels. Variety of rock crystallographic textures and its correlation with physical mechanisms of texture formation processes gives the key to establish the analytic methods for reconstruction of geological evolution factors. Relations between textures of various mineral phases of rocks and physical and chemical mechanisms of metamorphism, magmatism, creep and plasticity are should be under the consideration.

Neutron diffraction is most suitable for measuring global textures of different phases simultaneously, particularly in coarse-grained polyphase rocks. Using neutron texture analysis in complex with geological, petrological and petophysical methods the experimental data on crystallographic textures of polyphase rocks from the different deep levels of lithosphere have been obtained. The main mechanisms of texture development in investigated samples were made clear by comparing results on texture simulations with experimentally produced textures and with textures in natural samples.

On the basis of rock texture determination, an information about character and degree of rock anisotropy was acquired which may help to explain the nature of seismic boundaries in the continental crust, as well as in the lithosphere as whole.

DECREPITATION OF FLUID INCLUSIONS IN MINERALS AS A CONTROL FACTOR FOR ABNORMAL INCREASE OF AN IONIC CONDUCTION OF CRYSTALLINE ROCKS UNDER HEATING

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Electrical conduction of crystalline rocks is provided by two alternative tools: impurities of graphite and\or sulfides are responsible for the electron conduction [1] whereas an intercrystalline and porous fluids promote the ionic conduction [2, 3]. Traditionally only two sources of fluids use to be taken into consideration: an external one is presented by hydrothermal streams, and interior one is supplied by hydroxyl-bearing minerals (mica, chlorite, amphibole etc.). Experimental study of fluid inclusions in a natural waterless rock-forming silicates sampled of the Kola Superdeep Borehole cores and of the crystalline massifs in neighboring areas have brought an unexpected information on a high ability of water sealed up into quartz grains as micro inclusions. Some types of metamorphic and intrusive endogenic rocks which crystallized at temperature of 600-900°C and pressure 2-7 kbar contain 10-40% of quartz, and the content of "impressed" water inclusions in quartz grains vary of 0,2 up to 1,6 ml per gram of solid matrix. As evaluated, a total water capacity of the "interior quartz reservoir" in a granite-gneissic massifs (about $1x10^9$ kg per 1 km^3) is comparable with a "hydroxyl reservoir" (5-20 x 10^9).

There is an essential difference in interaction between the intergranular\porous fluids and the interior mineral water reservoirs. Hydroxyl group (OH) is installed in a crystal structure and could be removed into the porous space only by complete destruction of host minerals. The exchange process performs an irreversible metamorphic dehydration, resulting in a transformation the water-rich rock types in their waterless homologies. In contrary to the dehydration, a water extraction of natural quartz "ampoules" does not need a destruction of the host crystals, because fluids emigrate of inclusion due to a decrepitation, which is the complex chain of microblasts in fluid inclusions and consequent transportation their contents through a rank of dislocation up to the grain surface. The process is reversible due to the host minerals are not ruined and so preserve an ability to catch and capsuled some portion of fluids from the porous space when temperature or stress in rocks will decrease.

That is necessary to emphases that additional portions of fluids generated by dehydration or decrepitation can produce an alternative effect on the ionic conductivity of a percolative fluid networks in the rocks. The dehydration use to produce a superpure water which increase a volume of liquid phase in the percolative network but contemporaneously an ion concentration in the liquid and a conductivity have to decrease. Otherwise, the decrepitation release from a closed ampoules in quartz and add to the percolative network a high concentrated natural electrolytes (content of NaCl into fluid inclusions can reach up 30-60%), and so the ionic conductivity of rocks have to grow up significantly. In the case study the abnormal increase of an electrical conductivity under heating of crystalline rocks was recorded at the temperature range 230-260°C when the mica is still stable and the "quartz reservoir" only was able to provide the reliable effect. As usual the quartz grains in rocks contain a series of inclusion with varying ratio gas\liquid, and the ratio can affect the temperature of decrepitation. That is give a key for explanation of appearance some peaks on a correlation curve "temperature vs. conductivity" in experiments on evaluation a conductivity of the quartz-bearing rocks under heating within temperature range 80-650°C.

AMPHIBOLITE ELASTIC PROPERTIES PECULIARITIES OF SD-3 GEOSPACE

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The studying of the Kola Superdeep borehole unique drilling materials represents a new stage in cognition of the deep continental Earth's crust down the Baltic Shield cross-section. The SD-3 geospace distinctive features are the medium anisotropy, stress and deformation complex fields and also the rock physical properties heterogeneity displaying as perpendicular so laterally.

Down the SD-3 the substantial genetic informativity deliver the amphibolites which portion in the SD-3 Archean cross-section makes up 30 %. The interrelation study of amphibolites and their host rocks, peculiariaties of their distribution as down the SD-3 so within its geospace and also the peculiarities of the inner composition of structures and textures have made it possible to single out two genetis classes – para- and orthoamphibolites. Longitudinal and lateral wave relatively low velocities under normal pressure and temperature and sharp velocity increasing with pressure rise are characterized for them. This phenomenon is explained by the closing of rock microfissuring having as natural so technogenic nature. The observations for the velocity change in time and their decreasing testify to the relaxation processes development connected to the microfissuring appearance that depends on rock bedding (Table).

Depth Interval	Vp_1 (1978) m/s	Vp_2 (2000) m/s	Δ V m/s
up to 8 km	4560	3400	1160
below 8 km	4620	3210	1410

It takes notice that the velocity anisotropy along the borehole axis is much low than the velocity anisotropy in the horizontal plane. Relatively low velocity anisotropy and amphibolite relaxation are most probably connected to these rocks deformation anisotropy accompanying by the dilatancy and the consolidated medium dispersion that is confirmed by the results of the neutron texture analysis. These processes mainly influence upon the wave field formation in the Earth's crust deep horizons.

Session "Neutron Activation Analysis for Life Sciences"

SPONTANEOUS CRYSTALLIZATION OF DIAMONDS IN A MELT OF METALS STUDIED BY NEUTRON-ACTIVATION ANALYSIS AND EPR

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Mechanisms of occurrence and growth of diamond crystals formed in the Ni-Mn-C system by the high-pressure and high-temperature (HTHP) method at T = 1650 K and P = 5,5 GPa are investigated. The phenomenon of periodicity of diamond growth after spontaneous crystallization is revealed during synthesis, with increase of share of a diamond phase in comparison with graphite.

With use of neutron-activation method of analysis in the synthesized crystals presence more than 20 chemical impurities from Na to W were identified and determined. The results show that concentration of impurities in the diamond crystals was from 1,5 – 0,1% (for Ni and Mn) to less then 0,1 ppm for W. It is established, that during growth of crystals, the content of elements varies according to factors of their distributions, relatives to factors of distribution of these elements in silicon. Some of these elements can enter during synthesis, interacting with each other (for example, Al and N), being allocated in an independent phase at disintegration of solid solution diamond-impurities. Transition of impurities and their complexes from crystals of diamond in melt and back is carried out as a result of processes of reorientation of crystals. It is established, that from all these elements the strongest influence on quality of diamond crystals renders capture inclusions of nickel and manganese, used as catalyst for diamond synthesis. Thus, at the initial stages of growth, these metals are grasped incoherent by growing together sites of growing faces of a crystal, and then, when growth of crystals becomes tangential – his edges and tops. It results in occurrence in crystals of strong internal stresses that are proportional to the inclusion concentration and which can be taken of due to stream own interstitial atoms. In particular, the irradiation of these crystals small dozes of neutrons results in appreciable decrease of internal stresses and, as consequence, to growth of hardness of crystals.

The results of investigation indicate that hardness of crystals during synthesis varies, achieving the maximal value after end of process of recrystallization and increases with the decreasing concentration of the substitutional nickel atoms.

AIR POLLUTION STUDIES IN CENTRAL RUSSIA (TVER', YAROSLAVL' REGIONS), USING MOSS BIOMONITORS AND NEUTRON ACTIVATION ANALYSIS

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The results of atmospheric deposition of elements in Tver', Yaroslavl' and the northern part of Moscow regions are presented. The data were obtained using the moss biomonitors technique and neutron activation analysis. The method of epithermal neutron activation at IBR-2 reactor of FLNP, JINR, Dubna has made it possible to determine the concentrations of major and trace elements over a large-scale range, from 10000 ppm for Mg, K, Ca to 0.001 ppm for Tb, Ta. Principal component analysis was applied to distinguish plant, crystal and general pollution components in the moss. The group elements, characterising pollution sources in these regions, were determined as well. There are: ferrous smelters (Fe, Zn, Sb, Ta); combination of non-ferrous smelters and plants (Mn, Co, Mo, Cr, Ni, W); the oil-refining plant and oil combustion at the thermal power plant (V, Ni). The obtained data are used to construct maps of element distribution over the investigated territory.

Source Evaluation of Metals in Minneapolis/St. Paul Metropolitan Area Road Surface Soils Using Principle Component Analysis

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Urban highway surface soils chemical contaminant levels are poorly understood. To fill in this data gap, the Minnesota Department of Transportation and the Joint Institute for Nuclear Research conducted a systematic surface soils geochemical survey in the spring of 2001 in the Minneapolis/St. Paul Metropolitan area Paul (Minnesota, USA). Using instrumental neutron activation analysis (INAA), wave-length X-ray fluorescence analysis (WL XRF) and flame atomic absorption spectrometry (FAAS) a total of 36 elements (Na, Mg, Al, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Br, Rb, Sr, Mo, Sb, Cs, Ba, La, Ce, Sm, Eu, Tb, Hf, Ta, W, Au, Pb, U, and Th) were evaluated in highway right-of-way and ambient background surface soils. Principal Component Analysis (PCA), a powerful tool to determine the relationships between chemicals and their pollution sources, was applied to these data sets. PCA found statistically significant relationships between As-Sb, Cr-Ni-Mo-W, and Zn-Pb indicating that each grouping could have originated from a similar pollution source. For example, the significant correlation of AS and Sb using PCA are typical findings for soils that have been contaminated by non-ferrous industry air emissions. Cr, Ni, Mo and W are characteristic for metallic dust due to abrasion of hard metal parts of cars. Zn-Pb found in highway right-of-way surface soils could originate from unidentified industrial sources. Observed lead in these surface soils may originate from past use of leaded gasoline (tetraethyl lead). Concentrations of two last groups of pollutants exhibit a nearly exponential decline with increasing distance from the highways.

AIR POLLUTION STUDIES IN R.MACEDONIA USING MOSS BIOMONITORING TECHNIQUE, NEUTRON ACTIVATION ANALYSIS AND GIS TECHNOLOGY

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For the first time the moss biomonitoring technique was applied to air pollution studies in the Republic of Macedonia, in the central part of the Balkan Peninsula.

Its mountainous and hilly relief, in spite of arid climate, was favorable for collecting terrestrial moss *Hypnum Cupressiforme*, *Campothecium lutescens*, and *Homolothecium Sericium*. Moss samples were collected in September-October 2002 in accordance with the sampling strategy of the European moss survey programme [1].

The sampling network included 73 sites evenly distributed over the territory of the country of 25713 sq.km). A total of 44 elements (Na, Mg, Al, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Zn, Ga, As, Se, Br, Rb, Sr, Mo, Ag, Cd, In, Sb, I, Cs ,Ba, La, Ce, Nd, Sm, Eu, Tb, Dy, Yb, Hf, Ta, W, Au, Hg, Th, and U) were determined by instrumental neutron activation analysis using epithermal activation at pulsed fast reactor IBR-2, FLNP JINR, Dubna, in the large-scale concentration range - from 10 000 ppm for Al and K to 0.001 ppm for some rare earths.

Principal component analysis (factor analysis) was used to identify and characterise different pollution sources and to point out most polluted areas. Six factors were identified. The interpretation of the factor analysis findings points to natural crust, marine, and vegetation components. Three other factors reflect anthropogenic origin of trace element deposition in the Macedonian moss samples: ferrous and non-ferrous industries, oil refinery, fertiliser production and central heating stations.

Four areas are experiencing environmental stress: Veles, Skopje, Tetovo and Kavadarci-Negotino, whereas agricultural south, south-west and south-east show median European values for most of heavy metals and other element-pollutants. GIS technology (geographic information system) is used for constructing black-and-white maps based on factor scores along with coloured maps of the distribution of some relevant elements for these factors over the investigated territory.

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ATMOSPHERIC DEPOSITION OF TRACE ELEMENTS IN ROMANIA STUDIED BY THE MOSS BIOMONITORING TECHNIQUE USING NAA AND AAS

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The first systematic study in Romania of atmospheric pollution from heavy metals and other toxic elements based on moss analysis was undertaken as a Romanian - Norwegian - Russian collaboration, primarily in order to assess the general situation regarding heavy metal pollution sources to the atmosphere in heavily industrialized parts parts of the country. An additional goal was to contribute to the European atlas of «Atmospheric Heavy Metal Deposition – estimation based on moss analysis» issued under the auspices of the United Nations Economic Commission for Europe in the framework of the International Cooperative Programme on Effects of Long-Range Transboundary Air Pollution. Samples of *Hypnum cupressiforme*, *Hylocomium splendens* and *Pleurozium schreberi* were collected in 1995-2001 at 294 sampling points (20x20 km network) in the Carpathian Mountains, Transilvanian plateau, and Prut river catchment. A total of 40 elements were determined using NAA and AAS. The total concentrations of antimony, arsenic, cadmium, chromium, copper, iron, lead, nickel, thorium, uranium, vanadium and zinc were determined and the results presented in the form of colored contour maps. Extremely high values were observed for As, Cu, Cd, Cr, Fe, Ni, Pb, Sb, Zn, and V in areas particularly affected by local industries. The heavy metal concentration ranges (in μg/g) in the examined areas were as follows: As (0.04-119), Cd (0.21-55.4), Cr (0.4-51.9), Cu (2.2-2423), Fe (471-21340), Ni (0.26-31.9), Pb (6.2-231), Sb(0.01-54), Th (0.06-5.3), U (0.01-1.36), V (1.9-54) and Zn (16.4-2946). These results are generally higher than those obtained in other countries of Europe using the moss technique. An attempt to establish a correlation of heavy metal pollution with health effects was undertaken in some areas of Romania.

MONITORING OF TRACE ELEMENTS AND RADIONUCLIDES AIR POLLUTION IN THE SOUTH URAL MOUNTAINS USING MOSSES AND SURFACE SOILS

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About one hundred samples of the mosses *Hylocomium splendens* and *Pleurozium schreberi*, collected in 1997-2001, were used to study the atmospheric deposition of heavy metals and other toxic elements in the South Ural Mountains (in some districts of the Chelyabinsk Region and in the southern part of the Sverdlovsk Region), characterized by intense anthropogenic impact from various industries including plutonium production – the source of radionuclides of great potential hazard. Samples of natural soils were collected at the 65 sites in order to investigate surface accumulation of heavy metals and to examine the correlation of elements in moss and soil samples to separate contributions from atmospheric deposition and from soil minerals. A total of 38 elements (Na, Mg, Al, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Rb, Sr, Zr, Mo, Sb, Cs, Ba, La, Ce, Nd, Sm, Eu, Gd, Tb, Dy, Yb, Hf, Ta, W, Au, Th, U) in soil and 33 elements Na, Mg, Al, Cl, K, Ca, Sc, V, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Br, Rb, Ag, Sb, Cs, Ba, La, Ce, Sm, Tb, Yb, Hf, Ta, W, Au, Th, U) were determined by epithermal neutron activation analysis. The elements Cu, Cd and Pb were determined in moss samples only by atomic absorption spectrometry. Special emphasis was made on the area affected by a copper smelter in the town of Karabash. The results were compared to those obtained by the authors for copper basins in Poland and Serbia as well as to baseline concentrations in Norway. VARIMAX rotated principal component analysis was used to identify and characterise different pollution sources and to point out the most polluted areas. ^{90}Sr and ^{137}Cs activity was measured in surface soil samples collected in 1998 beyond the Eastern Ural Radioactive Trace (EURT) in the northern part of Chelyabinsk Region, adjacent to the «Mayak» plutonium production association. The results obtained were combined with data from a previous study by the Danish-Russian collaboration based on samples collected between 1990 and 1995 within the EURT. GIS maps of the pollution patterns of the above radionuclides as well as maps of factor scores for heavy metals were created.

NAA AND AAS OF MOSS SAMPLES USED TO STUDY AIR POLLUTION IN THE THRACE REGION, TURKEY

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The moss biomonitoring technique was applied to study air pollution in the Thrace region, northwest Turkey, covering an area of 23764 km^2. This is the first reported application of this approach in Turkey. Moss samples *(Hypnum cupressiforme)* were collected from 54 sampling sites according to the guidelines of the European project on biomonitoring of atmospheric deposition [1]. Two complementary analytical techniques, epithermal neutron activation analysis (ENAA) at the pulsed fast reactor IBR-2 in JINR, Dubna, Russia, and flame and graphite furnace atomic absorption spectrometry (AAS) at NTNU, Trondheim, Norway, were used to determine a total of 43 elements including most of heavy metals and rare earths: Na, Mg, Al, Cl, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Br, Rb, Sr, Mo, Ag, Cd, Sb, I, Cs ,Ba, La, Ce, Nd, Sm, Eu, Tb, Dy, Yb, Hf, Ta, W, Au, Pb, Th, and U. Results obtained for Mn, Ni, Zn, and As by both methods are discussed. VARIMAX rotated principal component analysis was used to identify and characterize different pollution sources and to point out the most polluted areas. For the elements reported to the European atlas [1] (As, Cd, Cr, Cu, Fe, Ni, Pb, V, and Zn) the median concentrations in the Turkish samples showed to be within the concentration ranges observed elsewhere in Europe. GIS technology was used for constructing maps of the distribution of element concentrations over the investigated area.

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Session
“Material Sciences”

SOME EXAMPLES OF ENGINEERING STRESS ANALYSIS AT PULSED NEUTRON SOURCES

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Some examples of the time-of-flight (TOF) neutron diffraction measurements of the applied and residual stresses in the industrial materials and components are presented. The reverse TOF technique realised at the High Resolution Fourier Diffractometer (HRFD) of the IBR-2 pulsed reactor is exploited to make the residual stress mapping in a welded ferritic steel plate and a shape welded austenitic steel tube. The problem of converting the phase lattice parameters in the multiphase system under load to strain/stress representation is discussed. An analytical formulation relating the phase applied stress - elastic strain responses in the axial (along the load direction) and transverse directions was applied to analyse the diffraction spectra obtained during in situ neutron diffraction stress rig experiments on the ENGIN instrument at the ISIS pulsed neutron facility from austenitic stainless steel with martensite phase plastically induced at the time of preliminary cyclic tensile-compressive loading on a servohydraulic testing machine.

"REAL LIFE" REACTOR MATERIAL PROBLEM SOLVED BY NEUTRON STRESS SCANNERS

V.L.Aksenov, A.M.Balagurov, D.I.Nikolaev, V.V.Sumin, and A.V. Tamonov

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We studied residual strains in tails for atomic reactors. Examples will be presented in this Conference.

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INVESTIGATION OF RESIDUAL STRESS STATE IN BIMETALLIC ADAPTER STAINLESS STEEL-ZIRCONIUM BY NEUTRON DIFFRACTION

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A bimetallic adapter stainless steel – zirconium is used in some structures of reactors RBMK channels. This adapter is a complex cross section cylinder (fig.1) with a steel outer layer and a zirconium alloy inner layer. The adapter is produced by vacuum sintering at the temperature 900° C. The steel thermal expansion factor is three times more than the zirconium factor and thus when the adapter is being cooled down a steel shell is compressing a zirconium part. At this some residual stresses arise inside a bimetallic joint and then they can be as a reason of an adapter destruction or cracks nucleation. The aim of this work is to investigate a residual stress state of stainless steel near a splice of a steel part and a zirconium alloy part.

Investigated regions are shown in fig.1 as "Cross Section A-B", "Cross Section 2" and "Cross Section 3". The practice shows the cross section A-B is the most dangerous in view of fatigue failure where so-called the first zirconium screw tooth exists.

This work was performed by neutron diffraction method at High Resolution Fourier Diffractometer (HRFD) at the IBR-2 pulsed reactor in Dubna, Russia.

The measured results of all three experiments are shown in fig.2.

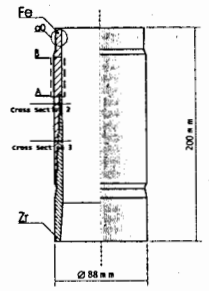

Fig.1. An adapter of reactor RBMK

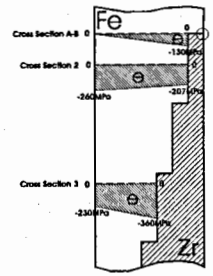

Fig.2. The scheme of the residual stress epures in a stainless steel in the various cross sections of the adapter. The wall of the adapter is shown in the area of the dangerous cross sections. The thin circle shows the stress concentrator.

Results:

1. The residual stresses in all three cross sections are the stresses of compression and it should salutary influence on the performance properties of the adapter, which works in enclosed tensile load conditions.
2. The analysis of the residual stress epures in the various cross sections allows us to draw a conclusion that the cross section A-B is the most dangerous from the point of view of fatigue failure of the adapter and the most probable place of the fatigue cracks origin.
3. In the two other cross sections 2 and 3 the situation is less dramatic. Values of the compression stresses are sufficient great allow to compensate the operational tension stresses on the internal surface of the adapter. Also an absence of any stress concentrators makes these cross sections as improbable places of the fatigue cracks origin.
4. We can create the more great compressive residual stress in the cross section A-B with the help of a corresponding heat treatment. This allows compensating a negative effect, which arises as a result of the stress concentrator existing in the given cross section. Moreover it allows compensating operation tensile load and accordingly it improves the residual stress state of the adapter, its operational characteristics and durability.

STRAIN SCANS ACROSS AN INTERFACE BETWEEN DUNITE AND QUARTZITE USING SYNCHROTRON AND NEUTRON DIFFRACTION

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In order to simulate meteoritic impact events a sample was made from two half-cylinders of dunite and quartzite. These half-cylinders were put into a steel tube, such that the polished surface of cut were in touch. As result of a shock wave deformation up to 37 GPa the two samples were joint together. Microscopic investigations show a few μm thick amorphous interface between the two minerals due to melting of dunite.

Synchrotron radiation was used for the strain investigations because its both good spectral (2θ) and spatial resolution (incident beam dimension $<0.2 \cdot 0.22$ mm). Furthermore, the high intensity of radiation shortens the required measuring time. For these reasons, the method is well suitable for small scale studies like profiling across borders between rocks or even grains. The investigations were carried out at the ROBL beam line of the ERSF Grenoble (France). In three levels with different distance from the bottom were made scans across the interface. Each scan had included 18 local positions for each mineral and covered a 2Θ-range of 4 degrees for the strongest peak.

At ISIS were carried out neutron time-of-flight strain measurements. The gauge volume was $1\times1\times5$ mm^3. By means of Rietveld method (GSAS) the deformation of the unit cells were found.

The striking result of the experiments with synchrotron radiation was the decrease of the peak intensity when approaching both the interface and the steel wall of the tube. The residual strain in the quartzite part is much higher than in the dunite part. The strain values obtained from neutron diffraction are in good agreement with those obtained from experiments with synchrotron radiation. The sizes of the crystallites were calculated from peak form analysis. First experiments were carried out for pole figure measurements using a 2d-detector and synchrotron radiation with short wavelength. The advantage of this new technique is an extremely short exposition time.

THE DYNAMICS OF IMPURITIES IN METALS STUDIED BY INELASTIC NEUTRON SCATTERING

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The results of dynamics investigation of the hydrogen and oxygen atoms in (Ta,V)-O and (Ta,V)-O-H alloys are presented for different temperatures and concentrations of impurities. The spectra of alloys vibrational states of the BCT lattice of β'-$VO_{0.2}$ were measured by inelastic scattering of slow neutrons (INS) at T=287K and T=19K. Alongside with local modes (LM) the gap-mode $\varepsilon\approx37$ meV is detected. The difference in the form of LM of oxygen at measurements with a creation and annihilation of a quantum of vibrational excitations is noted.

The investigations of the α-solid solutions of TaO_X by the methods of high-temperature quenching are executed. The results on dynamics of oxygen in Ta are obtained at 500K. The gap vibrational mode in $TaO_{0.024}$ ($\hbar\omega\approx33$ meV) is fixed. At the same time we can't establish reliable the energy of high-frequency mode in this system even at 500K. This fact alongside with the difference in the form of LM of oxygen at measurements with a creation and annihilation of a quantum of vibrational excitations is discussed.

In ternary alloys V-O-H it is shown that the hydrogen occupies different positions according to p-element concentration in metals. In β'-phase V-O-H the hydrogen remain into the almost ideal tetrahedral position up to temperature of liquid helium.

The energy and width of spectra of oscillations of hydrogen and oxygen, constant of force-interaction Ta-H and Ta-O, position of localization of hydrogen in solid solution Ta-O is determined. In a system Ta-O-H, as well as in Ta-H, the hydrogen occupies tetrahedral interstices practically not deformed by interaction H-O.

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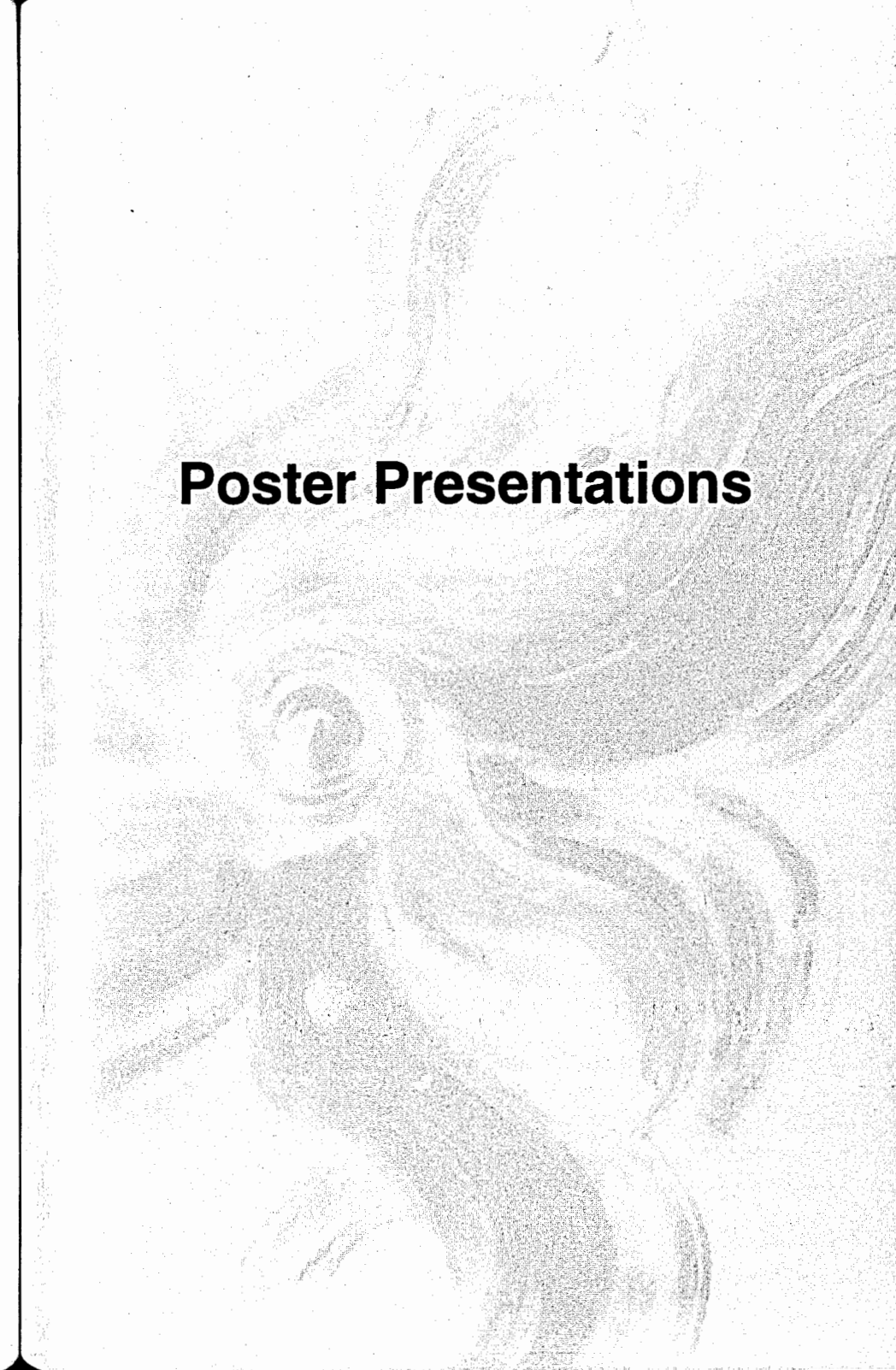
Poster Presentations



Session
"Cold Moderators"

CRYOGENIC IRRADIATION FACILITY URAM-2 AT THE IBR-2 REACTOR FOR RADYOLYSIS STUDY

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The irradiation facility URAM-2 was constructed for study radiolysis effects by fast neutron irradiation in some suitable for effective cold neutron production materials (namely: solid methane, methane hydrates, water ice, mesitylene and other). It has been designed and constructed in JINR and mounted at channel #3 of the IBR-2 reactor.

The cooling system of the facility is based on liquid helium as a coolant material. Samples could be loaded by condensing gas into irradiation cavity or by delivering and charging prepared before beads of ice or any low-boiling liquid into irradiation capsule. The large helium Dewar vessel gives opportunity to realize long time experiments. Some thermocouples are using for measuring temperature of: a sample, input and output helium, walls of the irradiation capsule.

Preliminary tests for each block of the facility and placing them at the working position were carried out in 2000-2001. The experiments for study of accumulation chemical energy under irradiation at low temperature (from 15 to 60K) and its spontaneous release during irradiation in mention above materials were performed from Nov. 2001 till Feb. 2003. The spontaneous reactions of radical recombination were observed by measuring the temperature jumps inside a sample and on the wall of the irradiation capsule.

The results of experiments are quite useful for development, optimization and construction of new advanced cold neutron moderators, both for the IBR-2M and advanced spallation neutron sources.

THE NEW WATER MODERATOR OF THE REACTOR IBR-2 WITH A CANYON ON THE LATERAL SURFACE. DESIGN AND PHYSICAL PARAMETERS

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An element of the new cold methane moderator of the reactor IBR-2, the water premoderator, serves as a thermal moderator for the 9th and 1st channels. Neutron radiation in the direction of the 9-th channel comes from the lateral surface of the moderator. A specific feature of the reflectometer REFLEX located on the 9-th channel is that it only "sees" neutrons emitted from a limited region of the moderator surface. This region is a rectangular extended along a vertical with a horizontal dimension of about 7 millimeters. To increase the flux on the sample, a groove-like pocket (canyon) with a depth of 80 mm by the width 15 mm and height 200 mm was cut in the premoderator on its lateral surface at 52 mm from the reactor core reflector. The design of the moderator and the results of measurements of the neutron flux distribution on the lateral surface of the moderator are presented in the paper.

THE EUROPEAN SPALLATION SOURCE FACILITY. VISION AND MISSION

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THE EUROPEAN SPALLATION SOURCE FACILITY. INSTRUMENTS AND LAYOUT

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Session "Neutron Instrumentation and Methods"

COMPLEX FOR MEASUREMENT OF DYNAMICAL CHARACTERISTICS OF NUCLEAR-PHYSICAL DEVICES

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For nuclear-physical investigations various dynamic and quasistatic magnetic fields, low temperatures and other hard conditions of experiment are used. Some devices require a precision angular orientation or a measurement of relative micromovings. In this connection the measuring-computer complex with replaceable Hall sensors has been developed at the Institute of Solid State and Semiconductor Physics of the National Academy of Sciences of Belarus. Such a facility allows to make a number of magnetometric and mechanoelectrical measurement.

During magnetometric measuring on the screen of the computer display three-dimensional components of a vector of a magnetic field induction are represented depending on time in situ, and then further mathematical processing of the received information is carried out.

The complex can be used for the determination of quasi-static and single pulse (the arbitrary form) as well as periodic magnetic fields by means of measuring three components of a vector of magnetic induction B_x, B_y, B_z .

The range of registered values of a magnetic field induction is 0,01–100 mT; 0,1–1000 mT; 1mT–10 T; the range of operating temperatures is 4,2–373 K.

The remote measuring block consists of three Hall sensors placed in three mutually perpendicular planes. Amplification of target signals of primary magnetic converters is realized by three two-cascade amplifiers. Two memory baseplates ADC 10M/12 having two synchronous channels (time of transformation is 100 nanoseconds; the RAM - 64 Kwords on the channel, an entrance range ± 2B, 4 lines of digital (TTL) input/output; external/internal synchronization, interruption, 14 digits) are built in a computer.

One-dimensional measurements in narrow backlashes up to 0,1 mm and deep apertures in diameter up to 0,75 mm are possible due to special sensors.

At mechanoelectrical measuring the signals from the precision angle of turn transmitter or linear displacement transducer which mode of functioning is based on Hall effect are used. So in angle of turn transmitters the transformation of an angle of shaft turn to an electric signal is made by Hall elements at rotation of two constant magnets around them. The pair of magnets creates the homogeneous magnetic field changing as sine-cosine law relatively to inter-perpendicular planes in which Hall elements are located. In contrast to transformer sine-cosine converters it is possible to make angle measuring at quasi-static and static turning angles to within the one tenth of angular second. Temperature correction is easily realized by the processor.

Applying plug-in linear displacement transducer with the help of the developed complex it is possible to measure the displacements by non-contact method with accuracy of 10 nanometers. At that the miniature magnetic system creating approximately a constant gradient of magnetic field induction moves relatively to Hall element (elements).

THE NEW HIGH INTENSITY NEUTRON TOF-SPECTROMETER AT THE MMF

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INSTALLATION OF HIGH HYDROSTATIC PRESSURE ON SMALL-ANGLE SPECTROMETER YuMO

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Installation of high hydrostatic pressure on small-angle spectrometer YuMO, capable to create pressure up to 4 kbar is created. The circuit of installation, basic elements, constructional features of the device are given. Curves of dispersion for lipidic membranes and micellar objects are received with the help of the chamber of pressure connected to installation. Measurements of the same samples in quartz a ditch "Hellma" are carried out. The sizes for connection of any other chambers of pressure and the basic characteristics of the device are given.

INELASTIC NEUTRON SCATTERING ON ACOUSTIC WAVES IN SOLIDS STUDIED BY NSE

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Inelastic neutron scattering (INS) by acoustic waves (AW) studied by means of NSE was recently described in [1]. For the case of perfect Si single crystals it was observed increasing of the diffracted beam total intensity, elastic scattering and the phonon harmonics up to n=7 as a function of the AW power. In deformed Si elastic scattering strongly decreases at the small AW amplitudes. These results are in agreement with dynamical theory calculations. At the highest power observed a crossover to a chaotic phonon behavior and rapid decay of NSE signal is described by model of quasi mosaic crystal. For the case of classical mosaic crystal KBr new secondary extinction effect was found. Mosaic block vibrates as a whole in the AW field. For moderate size of mosaic blocks secondary extinction for the elastic scattering and INS should be considered separately and ultrasound leads to the increasing of the total intensity of scattering. Results of secondary extinction calculations are in a good agreement with the results of our NSE experiment with KBr and mica. Also INS was observed in the strongly excited pyrolitic graphite and even in quartz glass where the effect of the AW at total intensity was absent. It is shown that NSE may be applied for acoustic wave studies in solids. Some conclusions about coherent or incoherent sound, AW modes in crystals and so on can be done.

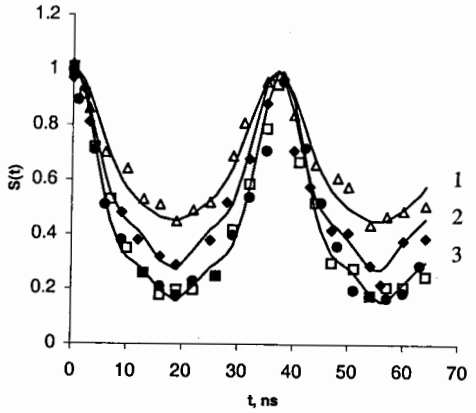

Fig. Normalized NSE signal for mica single crystal. λ_n = 1.102 nm. Generator voltage: 1-100 mV, 2 - 150 mV, 3 - 200 mV. Ultrasound frequency - 28 MHz. Solid curves – fitting:

$$S(t)=\sum_{n=0}^{n=\infty}A(n)\cos(2\pi n f_S t),\quad S(0)=1$$

f_S is the frequency of ultrasound generator. Cosine Fourier transform S(t) allows to find probability A(n) of the n-phonon scattering and its dependence from the AW amplitude (generator voltage).

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NEUTRON REFLECTION FROM AN ULTRASONICALLY EXCITED LAYERED STRUCTURES AND GLASS MIRROR

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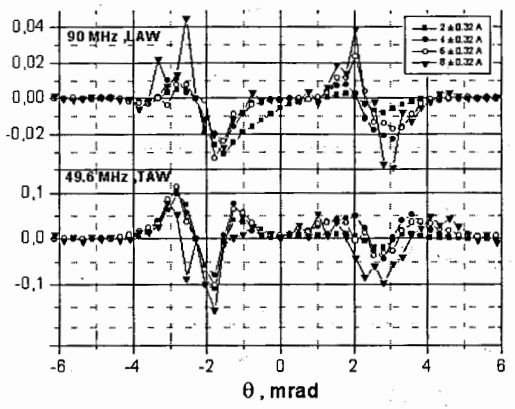
The regimes of total and Bragg reflection of polarized neutrons from a layered structure are investigated as a function of the amplitude and frequency of transverse (TAW) and longitudinal ultrasonic waves (LAW) excited in the structure. Measurements were carried out by spectrometers PNS-1 and REFLEX (Dubna) and V-6 (Berlin) The off-specular reflection of neutrons and the shifting of the nodes and antinodes of the neutron wave field are observed.



Also the neutron reflection from a glass mirror is studied in the same regimes. The off-specular reflection of neutrons due to energy exchange between the neutron and the sonic wave that occurs with a low probability is investigated. In the region of total neutron reflection the intensity of the off-specular reflection of neutrons from the mirror is a periodic function of the neutron wavelength. Some results for glasses are shown on Fig. It is clearly seen effect is large, reaching for TAW and decreasing reflection intensities more than 10%. This data correspond to theory developed recently in [1].

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NEUTRON DIFFRACTION BY ACOUSTIC WAVES IN PERFECT AND DEFORMED SILICON CRYSTALS

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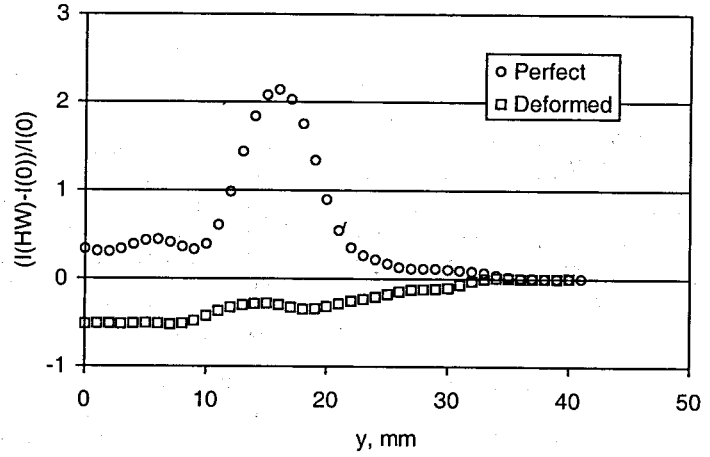
Recently theoretical, experimental and numerical analysis of the effect of acoustic vibrations on neutron diffraction in slightly deformed Si single crystals was presented. The measurements were made in Laue and Bragg geometries High frequency ultrasonic waves in slightly deformed silicon single crystals strongly influences on the neutron diffraction. This effect increases when the neutron acoustic resonance conditions are fulfilled. Experimentally it was shown that the deformation parameter **B**~0.03 can be measured and this value corresponds to the lattice relative



deformation $\Delta d/d \sim 10^{-6}$. The difference between ultrasound effects in perfect and deformed Si single crystals is clearly seen on Fig., where relative diffraction intensities for 14,8 MHz ultrasound (I(Hw) is beams intensity with sound , I(0) – without) obtained in the scanning procedure. The another difference is two new types of oscillations: sound extinction beating for perfect crystal and "deformation Pendellosung" for slightly bended silicon.

THE RESOLUTION FUNCTION FOR A PULSED-SOURCE TOF NEUTRON SPECTROMETER WITH MECHANICAL MONOCHROMATOR

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The concept of resolution function has been first introduced by Nathans&Cooper in 1967, [1]. The proposed computational method, involving only angular variables, is suited only for rather simple configurations as the conventional double and triple axis spectrometers are.

The matrix procedure first proposed by A.D.Stoica in 1975, [2], is suited for a large variety of experimental configurations, [3], [4], [5], [6], in particular for sophisticated ones using the focusing effects where spatial effects are important, [7], or for TOF instruments.

The Monte Carlo procedure requires computers with increased memory and computing speed while, for the matrix method, a normal 486 PC is quite suited, with computing times of 1-2-seconds. Therefore the matrix method should be preferred. If a precise description of the line profile is needed, the M.C. procedure should be used.

The general theory for the matrix method is briefly given. The application of this method for a pulsed-source TOF neutron spectrometer with mechanical monochromator is then given.

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DEVELOPMENT OF THE SOFTWARE COMPLEX FOR THE YUMO SPECTROMETER AT IBR-2 REACTOR

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In 1999 the old YuMO spectrometer control system base on PC and CAMAC was replaced with the VME computer. As a result the MS DOS instrument control program was also replaced with the new software complex. The report is devoted to the result of this modernization. The main features of the new software are described. A comparison between the old and the new ones are presented. It is shown that new software is more powerful, flexible and stable than the old system.

AUTOMATION AND ENVIRONMENT OF A SAMPLE OF MODERNIZED INSTALLATION YUMO

Sirotin A.P., Volodin O.V., Gordelij V.I., Islamov A.H., Kovalev J.S., Kulik V.D., Lazin V.I., Petuhova T.B., Smirnov A.A., Utrobin P.K. and Kuklin A.I.

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The new potential of modernized installation YuMO is shown due to automation of separate units. Advantages of a new condition of a spectrometer are shown. The basic approaches to creation of control systems by executive mechanisms of spectrometers on a basis are formulated.

Circuits of the block of management by step-by-step engines, the switchboard - amplifier of step-by-step motors, the circuit of system of stabilization of the period and a phase of the chopper, and the block diagram of a control system of executive mechanisms of spectrometer YuMO are submitted. Descriptions of the basic original mechanical devices are given.

THE APPLICATION FOR INITIAL PROCESSING OF SMALL ANGLE SCATTERING SPECTRA

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The SAS application is intended for processing of the spectra measured on installation MURN on the channel number four of the IBR-2 reactor. This program allows to combine data concerning the same sample, to calculate resolution function of the installation for the given conditions of experiment, to carry out correction of the data on dead times of detectors of the neutrons and to subtract a background substrate from the detector's data in two possible modes: with using of the breaker of a beam of neutrons or without it, to carry out normalization of the received spectrum on independent (standard) vanadium scatterer, to subtract the data of the background samples.

SOFTWARE FOR NEUTRON ACTIVATION ANALYSIS AT REACTOR IBR-2, FLNP, JINR

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A Delphi program suite, developed for processing gamma-spectra of induced activity of nuclei, obtained from the neutron activation measurements at the reactor IBR-2, FLNF, JINR, is reported. This suite contains components, intended for carrying out all the operations of the analysis cycle, starting with a data acquisition program for γ-spectrometers Gamma (written in C++ Builder) and including Delphi programs for the following steps of the analysis itself:

1. VACTIV, which performs the automatic robust least-square fitting of the spectra and extracts such characteristics of interest as energies and intensities of lines of the activated sample.
2. Ist, which performs qualitative analysis of the sample - identification of sample isotopes.
3. NewMass, which performs quantitative analysis - determination of concentrations of the identified isotopes in the sample.
4. NewDig, which forms different information and reference tables on the basis of the analysis results.

The following goals were persecuted while developing these programs:

1. Implementation of the new programming techniques – visual object-oriented languages and graphical dialog, which enables us to supply the user with a very convenient and friendly interface.
2. Creation of very efficient tools for the analysis of gamma-ray spectra: algorithms are independent of peak shape, that is the unique property of the program; include a large variety for automatic peak search; the least-square fitting is very fast and efficient due to the use of different methods for robustness and damping of ill-conditioned matrices, etc.
3. Specific attention was focused on problems of analysis sensitivity and resolution - determination of statistical limits, which guarantee the reliability of parameter estimates and inference, based on them.

The program suite runs in any Windows-XX environment and enjoys all the benefits of these operating systems. Now it has become a routine instrument in the NAA experiments on studies of ecological, biological, geological etc. samples.

BANK OF SCIENTIFIC INFORMATION

G.M.Mironova

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More than 1000 physical processes followed in real time on the DN-2 diffractometer at the IBR-2 have been accumulated in the Bank of Scientific Information (Dubnainfo) in digital and colour object presentation. The key features of these data are unprecedentedly short exposures (1-300 pulses of IBR-2), unprecedentedly large simultaneously covered detector angle range (0-179 degrees) and largest range of incoming neutrons (1-25 A). The physical processes at different temperature regimes include reduction and oxidation phenomena, chemical reactions and phase transitions, setting and dehydration of cement pastes, melting and solidification of some compounds, etc. This unique data collection allows us to understand fundamental phenomena in chemistry, physics, geology, biology, astrophysics.

FIT A CHOSEN THEORETICAL MULTI-PARAMETER FUNCTION THROUGH A SET OF DATA POINTS

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Fitter 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 disigned to be used for a small-angle neutron scattering data analysis. Respective theoretical models are implemented in it. Some common used models (Gaussian and polynomials) are also implemented for wider aplicability.

Session

"Condensed Matter Physics - 1"

SANS INVESTIGATIONS OF MICROSTRUCTURAL CHANGES IN SOL-GEL DERIVED IRON OXIDE/SILICA MATRIX NANOCOMPOSITES

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[b]*Joint Institute of Nuclear Research, FLNP, Dubna, Russia*
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Porosity and grain size generation in nanometer scales is a crucial factor for most of applications [1]. The sol-gel method appears to be particularly attractive to achieve these objectives since the process is carried out in a liquid phase, at near ambient temperatures, with the additional positive effect on the overall energy consumption and environment.

The use of a porous inorganic matrix provides spatially localised sites for nucleation and minimises the degree of aggregation of the iron oxide particles.

Presently, there is a great interest in synthesis of iron and iron oxides particles embedded in silica matrix that have potential application to information storage, sensors[2-4], magnetic refrigeration, and magnetic resonance imaging enhancement.[5-7] There is necessary to be studied metal ions entrapped in porous silica sol-gel matrices, fractal dimensions, defect formation and defect structure evolution in maghemite, temperature of maghemite-hematite transformation, porosity of the silica matrices to reveal new aspects of the physical nature of composites and thus to direct the way to increase their thermal stability. In the present paper nanosized silica matrices and nanocomposites (consisting in α- or γ-Fe_2O_3 particles confined in porous silica matrix) were characterised by Small-Angle Neutron Scattering, SANS.

Experimental data, concerning nanoporous sol-gel derived materials (sonogels and xerogels, iron oxide silica nanocomposites) structure (texture) previously obtained by different characterisation techniques (electron microscopy, X-ray diffraction, Mossbauer Spectroscopy), and SANS experiment results are presented in order to obtain a consistent picture of investigated objects in nanometre scales, from different perspectives.

The SANS preliminary measurements were overdone at the facility in function at IBR-2 pulsed reactor in Dubna. The Q values covered in these measurements ranged from 0.005 to 0.37 $Å^{-1}$. In Fig.1 the SANS scattering curves in log-log plot of IOS1-IOS11 silica xerogel (IOS1, IOS8) and iron oxide embedded in silica matrix samples are presented.

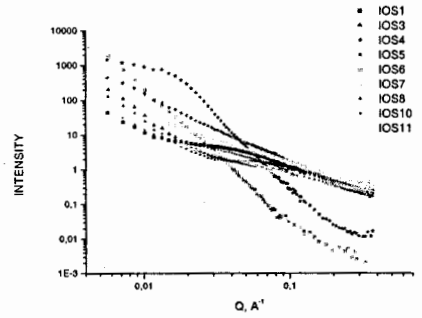

Fig. 1. SANS curves of IOS1-IOS11 samples

Calcination is expected to eliminate organics and causes smoothness of the surfaces of samples and shrinkage of the xerogel backbones. Appearance of new pores due to pyrolysis of organics, shrinkage of backbones or collapse of pores would have the effect of making coarser surface. So increase of D_m can be attributed to the elimination of remainder TEOS, shrinkage of the gel backbone or collapse of pores although smoothness might also occur, while the decrease of D_m indicated that the smoothing of surface prevails [8].

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MIXTURE SYSTEM FOR TRITONX-100+SDS (NONIONIC + ANIONIC CLASSIC SURFACTANTS) STUDY BY SMALL ANGLE NEUTRON SCATTERING METHOD

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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 system of nonionic classic surfactant TritonX-100 and anionic classic surfactant SDS (sodium dodecyl sulfate) in water solution was investigated for temperatures 30°, 50°, 70° C (Fig.1) for compositions TX-100+SDS (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 $8x10^{-3}$ to 0.4 $Å^{-1}$.

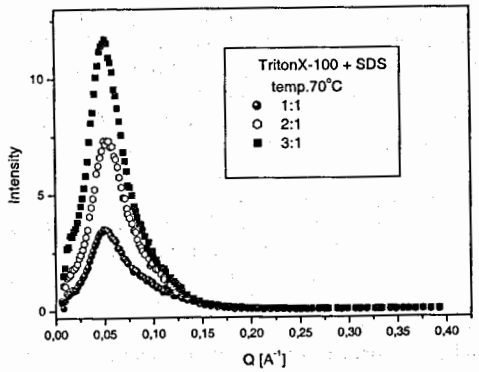

Fig.1. Differential neutron scattering cross sections for 1/1, 2/1 and 3/1 solutions in D_2O at 70°C.

The SANS measurements of aqueous solutions of nonionic / ionic surfactants have shown that the mixed micelles are formed. From the measured dependence of the scattered intensity on the scattering angle, we derived the aggregation number and the electric charge of the mixed micelle at various compositions and ionic strengths. The size of mixed micelle is a weak function of the mixing ratio between the two components.

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STRUCTURAL ANALYSES OF COMPOSITE MATERIALS WITH NANOCARBON AS FILLER

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The carbon composite materials are now one of the major structural materials for many industrial applications because they present a lot of advantages over other structural materials. Among them are the following: at high-temperature the mechanical properties don't change much; they posses a low density, a low coefficient of thermal expansion, as well as a good electrical conductivity, etc.

The coal tar pitch is a suitable precursor for preparation the advanced carbon material with controlled properties. The heat treatment of the coal tar pitch leads to more organized and staked arrangement of the aromatic sheet that can form a separate liquid-crystal like phase known as carbonaceous mesophase. The later has a spherical morphology, which arises, grows and manifests the coalescences during the heat treatment and forms a paracrystaline carbon structure close to that of graphite. The texture of mesophase is strongly controlled by rheological properties, temperature and the heating rate during the heat treatment, as well as the quantity and type of additives, which can inhibit or catalyze the formation, growing and coalescence of the mesophase spheres.

The embedding of the conductive particles into a polymer matrix modifies fundamentally the electrical conductivity of the composite. The polymer matrix can become a semiconductive or conductive material, when it is doped with conductive additives.

The aim of our work is to design and develop this kind of composite material for EMI shielding and other electrical, chemical and biochemical applications.

This paper presents the results of complex investigations of structural modifications induced during the heat treatment at 440^0 C and 900^0 C in the coal tar pitch by adding different quantity (0.1, 0.5, 1 weight %) of nanocarbon.

They include studies of optical and electronic microscopy, x-ray diffraction, Raman spectroscopy and small-angle neutron scattering.

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CHARACTERISING OF LOCAL ORDER IN AQUEOUS SURFACTANT SOLUTIONS BY SANS AND THERMODYNAMICS METHODS

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MOLECULAR MOTIONS IN ETHYLENE GLYCOL: QUASIELASTIC NEUTRON SCATTERING STUDY

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The results of the neutron scattering experiment on ethylene glycol (H-O-CH_2-CH_2-O-H) at T=300K, T= 348K and T = 393 K by using "direct geometry" double time-of-flight neutron scattering spectrometer DIN-2PI (Frank Laboratory of Neutron Physics, JINR, Dubna) are presented. Measurements were performed with incident neutrons energies E_0 = 2meV (with an elastic resolution ΔE = 90 μeV) and E_0 = 3meV (ΔE = 160 μeV). The reorientation and translation components of the quasielastic scattering are investigated. A very broad reorientation component (~ 1 meV at T = 348K) is observed, which is supposed to be connected to the rotation motions of protons of weakly polar methylene groups. The data processing is still in progress and further results will soon be available.

MAGNETIC STRUCTURES OF $NDMNO_3$ CONSISTENTLY DOPED WITH SR AND RU

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The crystal and magnetic structures of the $(Nd_{1-x}Sr_x)(Mn_{1-x}Ru_x)O_3$ perovskites have been studied by neutron powder diffraction. The simultaneous and consistent doping of the A- and B-sites with Sr and Ru has been used for avoiding the Mn^{4+} formation and hence, suppression of the double exchange. All studied samples ($0 \le x \le 0.875$) are insulators and show unusual long-range ferromagnetic state with antiparallel ordering of Mn and Ru magnetic moments. We conclude that ferromagnetism in this doped compound is not caused by the double exchange; nevertheless this interaction is important for correlation between ferromagnetism and metal conductivity.

NEUTRON POWDER DIFFRACTION STUDY OF $La_{0.67}Ca_{0.33}Mn_{1-x}Fe_xO_3$ (x=0, 0.3, 0.9)

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Neutron diffraction measurements were performed on the high-resolution powder diffractometer "Mini-SFINKS" utilising the reverse time-of-flight Fourier (RTOF) method [1] at the WWR-M research reactor of the Petersburg Nuclear Physics Institute. These measurements covered the temperature range 20K≤T≤300K and the interplanar distances 0.5Å≤d≤2.7Å.

The patterns obtained were analyzed by the Rietveld method with the profile refinement program MRIA [2]. Following structural parameters were varied during the refinement procedure – lattice parameters a, b, c; coordinates of the La (Ca), Mn (Fe), O atoms x, y, z; extinction parameters (effective sizes of mosaic blocks); thermal parameters of atoms in the isotropic approach β_{isotr}.

The values of the lattice parameters indicates that the structure of all samples at the whole temperature range is characterized by the relation $c > a > b/\sqrt{2}$. The rombohedrical lattice distortion is rather significant – about 0.15%. As it has been shown [3], changes in values of the parameter c are connected with changes in magnitudes of the tilting octahedral distortions, whereas changes in values of the parameter a are a good indication of magnitudes of the cooperative JT distortions. The relation c > a, contrary to the well-known in manganites orthorombical distortions O- and O'- types, pointes to the distortion of the O2-Mn-O2 angles of the octahedral, which lies (as a rough guide) in the basic ac plane. The values of the Mn-O bond lengths in the whole temperature range indicate very small cooperative JT distortions.

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STRUCTURAL AND MAGNETIC PHASE TRANSITIONS IN $RbMnCl_3$

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The family of crystals ABX_3 (A one-valent, B bivalent, X - F, Cl, O) attracts attention of researchers an abundance of crystal and magnetic structures, variety of types of phase transitions. Here crystals with perofskite-like structure in which phase transitions of different types are observed, most are investigated.

Crystal $RbMnCl_3$ at reduce temperature tests two phase transitions:

$$G_0 \rightarrow G_1 \rightarrow G_2$$

At room temperature $RbMnCl_3$ has hexagonal symmetry (phase G_0 = $P6_3/mmc$, a=7.161, c=17,831 Å, γ =120°). At reduce temperature it undergoes structural phase transition and is lower 270 K becomes monoclinic (phase G_1). Existence structural phase transition for the first time is revealed in work [1], at optical research in the range of temperatures from room up to 100 K.

The further reduce of temperature results in formation of an antiferromagnetic condition (phase G_2). Neutron researches which have been carried out Melamud and Makovsky [2] in a temperature interval from 4.2 up to 300 K have shown that magnetic and chemical elementary cells are equal, and the magnetic structure represents a set of ferromagnetic layers of atoms Mn, which are connected antiferromagnetic. Neel temperature for $RbMnCl_3$ is equal 94.6 K. However, existence of structural phase transition in this work was not revealed, and magnetic cell description was carrying out in assumption hexagonal crystal structure.

Results of crystal and magnetic structure research of $RbMnCl_3$ by a method of neutrons diffraction are submitted in the report.

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STRUCTURAL STUDY OF MANGANITES $Pr_{1-x}Sr_xMnO_3$ (x = 0.5, 0.56) AT HIGH PRESSURE

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Crystal and magnetic structure of manganites $Pr_{1-x}Sr_xMnO_3$ (x = 0.5, 0.56) in the pressure range up to 4.5 GPa and temperature range 16 – 300 K has been studied by means of powder neutron diffraction. At ambient pressure, both compounds have a tetragonal structure (sp. gr. I4/mcm). In $Pr_{0.5}Sr_{0.5}MnO_3$ at T_C = 265 K a phase transition from paramagnetic to ferromagnetic (FM) metallic state occurs. At T_N = 155 K it transforms to A-type antiferromagnetic (AFM) state and this change of magnetic state is accompanied by the structural transformation to an orthorhombic structure of sp. gr Fmmm. In $Pr_{0.44}Sr_{0.56}MnO_3$ at T_N = 217 K a phase transition from paramagnetic to A-type AFM state occurs which is also accompanied by the structural transformation to the orthorhombic structure of Fmmm symmetry.

At P = 1.9 GPa in $Pr_{0.44}Sr_{0.56}MnO_3$ and P = 3.2 GPa in $Pr_{0.5}Sr_{0.5}MnO_3$ an appearance of C-type AFM state was observed on cooling and both A-type and C-type AFM state coexist at T = 16 K. In $Pr_{0.5}Sr_{0.5}MnO_3$, an effect of high pressure leads to a suppression of FM state and increase of a transition temperature (T_N) to A-type AFM state. While at ambient pressure and T = 200 K a pure FM state in $Pr_{0.5}Sr_{0.5}MnO_3$ was observed, at P = 1.9 GPa and T = 200 K the only A-type AFM state was observed and nearly no FM contribution. Structural parameters of $Pr_{0.44}Sr_{0.56}MnO_3$ and $Pr_{0.5}Mn_{0.5}SrO_3$ as functions of pressure were obtained.

The work has been supported by the Russian Foundation for Basic Research, grant 03-02-16879 and Russian Ministry of Science, Industry and Technology, State contract № 40.012.1.1.1148 and grant of support of unique facilities of Russia.

COEXISTENCE OF SUPERCONDUCTIVITY AND FERROMAGNETISM IN Fe/V BILAYER

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Coexistence of superconductivity and ferromagnetism in layered FM/S structures results in influence of magnetism on superconductivity and influence of superconductivity on magnetism [1]. In theory, competition between one-dimensional (1D) and three-dimensional (3D) Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) states is considered now. As result, two-dimensional wave vector q_f exists in the plane of ferromagnetic layer and there is its dependence on exchange field magnitude. From that, heterogeneity of a magnetic induction is supposed and thus spin-flip process and diffusion scattering of neutrons are predicted. Polarized neutron reflectometry measurements have been carried out with samples MgO/[5nm Fe/5nm V]$_{10}$/[0.145nm Fe/0.145nm V]$_{17}$/40nm V/1.5nm Pd and MgO/[3nm Fe/3nm V]$_{20}$/3nm Fe/40nm V/1.5nm Pd at temperatures 1.6, 3, 7K and external magnetic field values 0.2, 0.7, 1.5-1.6 and 4.5 kOe. The spin-dependent neutron reflection was observed at transitions of the samples in superconducting state: nonmonotonic dependence on temperature for the first sample and distinctions depending on magnitude of a magnetic field for both samples.

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POLARIZED NEUTRON REFLECTOMETRY STUDIES OF NUCLEAR AND MAGNETIC PROFILES IN FE/V LAYERED STRUCTURES

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Polarized neutron reflection from the surfaces and interfaces of magnetic layers does supply information about nuclear and magnetic structures. In this report we give the results of the polarized neutron reflectometry studies of MgO(001)[^{57}Fe(20ML)V(14ML)]$_{20}$Pd and MgO(001)[^{57}Fe(7ML/V(10ML)]$_{29}$ Pd structures and present their nuclear and magnetic depth profiles. From fitting of the experimental extracted nuclear and magnetic depth profiles and model calculations, based on real boundary interface, the conclusion about antiferromagnetic ordering of vanadium and iron near to the interface follows. Neutron measurements were performed at spectrometer REMUR of IBR-2 reactor in Dubna.

INVESTIGATIONS OF RESIDUAL STRESSES FOR THE NUCLEAR INDUSTRY CARRIED OUT AT FLNP JINR

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Residual stresses are stresses, which exist inside some solid body at absence of any kinds of external forces and temperature fields. As usual, these stresses arise in details due to various manufacturing processes and as consequence they exist practically in all details and constructions. Nowadays designers and engineers can analyse a construction for durability, but they can't take into account that technological processes of manufacturing have created rather great residual stresses in a detail. Therefore, it is absolutely necessarily to posses methods which would allow to measure residual stresses in details after all technological processes of manufacturing. One of such methods is the high-resolution neutron diffraction.

Two special time-of-flight diffractometers are used for residual stress measurements at IBR-2 pulsed reactor in FLNP JINR (Dubna, Russia). These are High Resolution Fourier Diffractometer (HRFD) [1] and Fourier Stress Diffractometer (FSD) [2] and their principle operation is based on an application of the reverse time-of-flight (RTOF) method – a kind of correlation technique – at long pulsed neutron sources. Such a way, high resolution in interplanar spacing ($\Delta d/d \approx 1\times10^{-3}$) can be achieved, while maintaining high flux at the instrument. The main advantage of the RTOF-method, as well as of the usual TOF-method, is the possibility of simultaneously measuring many reflections, which allows to determinate the residual strains along various (hkl) directions in a crystal. Moreover, the HRFD resolution function has rather simple dependence on interplanar spacing d, which allows one to easily estimate microstrain averaged on all (hkl) directions from analysis of width of several diffraction peaks.

Nowadays, all necessary equipments for a such an experiment are available. There are the linear scanner, 5-axis goniometer "HUBER" for a measurement of the full residual strain tensor, the loading machine "TIRA-test" for in-situ experiments and definitions of materials elastic properties, a mirror furnace for an investigation of materials at high temperatures (up to 1000°C). All of these devices can be used simultaneously that allows expanding experiment's opportunities and for example allows defining the dependence of material elastic properties on temperature etc.

On this work are also presented the results obtained from residual stress measurements carried out at FLNP JINR on various materials and details for nuclear science and engineering.

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STRUCTURE AND PROPERTIES OF THE NANOCRYSTALLINE IRON-BASED ALLOYS

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Investigation of the alloys with a small grain size (1--10) nm has lately been paid to much attention. This is due to a number of unique mechanical and magnetic properties that are peculiar to these alloys. Of special interest are nanocrystalline alloys, which represent record magnetic alloys, such as iron-based alloys with silicon and boron. The procedure of manufacturing these alloys is as follows. First, these materials are produced in the form of an amorphous ribbon by rapid quenching from the melt onto a rotating drum. Then, they undergo nanocrystallizing annealings at a temperature of 510-570°C. The heat treatment results in essentially changing the magnetic properties (coercive force, the type of magnetic anisotropy and its-constant magnitude). The rate of the processes significantly increases under action of stresses or a magnetic field that are applied in the course of nanocrystallizing annealing. Moreover, the temperature and duration of the heat treatment, the magnitude of a load, the strength and direction of an external magnetic field affect the changes as well. These processes are known to give rise to a complicated structural state of the alloys. To ascertain the relation between the magnetic state and structure formed in nanocrystalline $Fe_{73}Si_{14}B_9Nb_3Cu_1$ alloys produced upon different conditions, we performed a combined study. On the one hand, we employed such locally sensitive methods as NMR and NGR, which allow controlling the character of changes in the contents of the phase constituents. Transmission electron microscopy was applied as well. On the other hand, for the first time, the method of neutron diffraction was used that makes it possible to analyze the magnetic and structural state formed on the average over the whole sample bulk. To examine the nanocrystalline-grain size, the technique of low-angle neutron scattering was applied. The report presents a complex analysis of the experimental data obtained by different techniques.

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HIGH-TEMPERATURE NEUTRON DIFFRACTION INVESTIGATION CRYSTAL STRUCTURE OF SOLID ELECTROLYTE CS_3PO_4

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Solid electrolytes with cesium-ion conductivity are attractive candidates for a great variety of applications such as electrochemical sensors, ionic engines, thermoemission generators, diaphragms for electrolysis of the molten cesium galogenides, systems of refining of the molten alkali metals, in particular for regeneration of the molten sodium used as a heat carrier in contours of reactors on atomic power stations.

At present, however, a number of cesium-conducting solids are rather limited and their electric characteristics are not high enough.

Recently conductivity of solid Cs_3PO_4 has been measured in wide temperature range. It was found that Cs^+-cation conductivity of pure cesium orthophosphate is rather high: $3{,}15 \cdot 10^{-2}$ $S \cdot cm^{-1}$ at 600°C. That is higher than for the most of the individual cesium compounds.

In order to make clear details of the ionic transport mechanism in solid Cs_3PO_4 neutron diffraction experiments were carried out. Crystal structure of Cs_3PO_4 was investigated at two temperatures. At room temperature it is orthorhombic. However in superionic area (at 600°C) it becomes cubic. So structure transition in cesium orthophosphate gives rise transition in superionic state.

The work was supported by State Scientific and Technical Program "Current trends in the physics of condensed media", trend "Neutron investigations of condensed media" (State grant № 40.012.1.1.11.50) and Russian Foundation of Basic Research (Grant 02-02-16406).

STRUCTURAL STUDY OF THE INFINITE-LAYER COMPOUNDS $SR_{1-x}LA_XCUO_2$ AT HIGH PRESSURE

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The infinite-layer compounds has been prepared under high pressure in strongly reducing atmosphare. The crystal structure of the infinite-layer compounds $Sr_{1-x}La_xCuO_2$ has been studied at high pressure up to 6 GPa using time-of-flight neutron difraction. Structural parameters as a function of pressure was obtained.

Work is supported by the RFBR grands № 00-02-17077, № 00-02-17370 and grant of support of unique instruments of Russia.

STRUCTURE ANYLYSIS OF NaX AND NaLSX ZEOLITES WITH METHOXY GROUPS BY POWDER NEUTRON DIFFRACTION

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Zeolites exhibiting regular structure which can be easily modified, are important candidates for this type catalyst and many laboratories try therefore to „tailor" zeolitic catalysts of the requested properties. Nature of acid or basic sites, their amount and distribution of their strength in the zeolitic lattice belong to the most important problem of surface chemistry. Non-destructive testing methods, mainly neutron diffraction are used for the structure determination of these zeolite samples. The fact that the powder materials can be measured in the stay which are similar considerations like in practice, is very important. Chemisorbed methyl groups were prepared in the structure by chemical reaction of methyl iodide with reactive sodium cations available in S_{II} and S_{III} positions of faujasites. Methyl cations CH_3^+ (methylium ions), evolved during reaction, react immediately with the lattice oxygen forming surface bonded methyl groups [1]. Changes in the distribution of structural sodium cations in the lattice after chemisorption of methyl cations has been detected. Neutron powder diffraction patterns were collected at temperature of 298 and 7 K on the KSN-2 diffractometer which is placed at the LVR-15 research reactor in Řež near Prague and which was equipped with close circuit liquid helium cryostat type CP-62-ST/5. Rietveld analysis of the neutron diffraction data of NaX samples [2] led to the complete set of the structural parameters for both the initial evacuated NaX and NaLSX samples and those with chemisorbed methyl species [3]. The structural analysis was treated in frame of Fd3 space group and we have determined the occupation numbers of cations and the location of CD_3 groups. Methylium ions are located in X faujasite at O_4 and O_1 lattice oxygen atoms. The location at two different sites correspond well with two observed ^{13}C MAS NMR signals at 54 and 58 ppm of surface bridging methoxyls. The occupation numbers of Na cations in chemisorbed NaX has been decreased for $S_{I'}$ and $S_{I''}$ in contrary to the increase for S_{III} in comparison with the initial NaX. S_{II} is practically fully occupied in both cases. Chemisorbed methylium ions in NaLSX are located in similar positions as in NaX at O_4 and O_1 but the Fourier maps of nuclear density are better developed due to higher concentration of Na cations and methoxy groups. Some distortion of the lattice was found in O1-T-O3 and O1-T-O4 angle.

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NEUTRON POWDER DIFFRACTION STRUCTURAL INVESTIGATIONS IN LND ON THE KSN-2 DIFFRACTOMETER IN ŘEŽ NEAR PRAGUE

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The crystalline structure of materials is fundamental to our understanding of their properties. In most cases it is necessary to determine the structural parameters or phase transition parameters of some perspective materials, which contain oxygen or hydrogen atoms among the heavy atoms. Then the neutron diffraction together with powder samples are advantegous to use to solve these problems. The powerful this application is pointed by means of the Rietveld analysis method for the neutron powder records data treatment. Powder, or more correctly polycrystalline matter, is a common state of solid materials. Classical crystallography requires the growth of large single crystals. But in many cases, single crystals cannot readily be grown, as was case for 90 K superconductor. Single crystal growth is also a method of purifying materials, and often the most interesting materials are not „pure". The structure of material at high temperature, where single crystals are usually grown, may not be the same at low or even room temperature. Certainly the technologist would much prefer to work with materials in their „natural", i.e. polycrystalline state.

Therefore, the research activities in the Laboratory of Neutron Diffraction (FNSPE CTU Prague) on the neutron diffractometer KSN-2, placed in Řež near Prague, are focused on neutron scattering for solid state physics and material science investigations. Applications to condensed matter cover the range of problems location of light atoms and cation distributions, magnetic structures and studies of phase transitions and texture. New instrumentation of our diffractometer (double bent Si(311) monochromator, the position-sensitive detector banks (P4 Reuter-Stokes)) improved the resolution to the $\delta d\backslash d = 0/002$ in the d-region from 1.4 to 0.075 nm, such as the neutron flux enhanced to about 2.5 times higher level, and allowed for investigation of samples with volume 4.5 times smaller. We will continue our investigations of some promising materials, e.g. structure and magnetic order in $Y_{1-x}Ca_xMnO_3$ (x=0.3 and 0.5)[1], study of the mixed-valence manganites $Pr_{1-x}Na_xMnO_3$ [2-4], structural dependence of the high-T_c $Y_{0.8}Ca_{0.2}Ba_2Cu_3O_y$ superconductors on the oxygencontents (Y ranges from 6 to 6.89) and zeolites (types Na-Y, Na-(H,D)Y, Na-X, Na-(H,D)X, chemisorbed: NaX+CD_3, NaY+CD_3. Experimental results of our investigations will be presented.

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THE EFFECT OF TH SUBSTITUTION ON THE CRYSTAL STRUCTURE AND THE CRYSTAL FIELD SPECTRUM OF THE HIGH-T_c SUPERCONDUCTOR $HoBa_2Cu_3O_{6.95}$

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In order to investigate the charge states in the CuO_2 planes of the high-T_c superconductor $HoBa_2Cu_3O_{6.95}$ induced by the in-plane electron doping, we studied the crystal structure and the crystal field (CF) effects for $Ho_{1-x}Th_xBa_2Cu_3O_{6.95}$ ($x \approx 0.07, 0.13$) by neutron powder diffraction and inelastic neutron scattering methods, respectively. As expected for the "negative" doping of the planes, increase in the Th^{4+} concentration decreases the lattice orthorhombic strain $s=2(b-a)/(a+b)$ while the lattice parameter c increases. Opposite to the case of the Ca^{2+}-doped $HoBa_2Cu_3O_{6.95}$ [1], partial substitution of Th^{4+} for Ho^{3+} does not result in the appearance of the additional spectral components in the CF spectra. Thus, we cannot identify optimally doped and underdoped domains in the system, similar to the case of the overdoped $Ho_{1-x}Ca_xBa_2Cu_3O_{6.95}$ in which the optimally doped and overdoped domains are found. However, some energy shifts and intensity variation of the observed CF transitions in the samples with Th^{4+} substitutions are compatible with an idea of charge carrier compensation in the CuO_2 planes due to electron doping. Decrease of the hole concentration in the planes with increase in x is confirmed by the bond valence sum calculations.

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MICROSCOPIC STRUCTURE OF LIQUID NA–PB ALLOYS STUDIED BY NEUTRON DIFFRACTION

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Neutron diffraction experiment on Na–Pb alloys allows to obtain data on microstructure of liquid sodium with lead impurity as surface-active inhibitor. This information will serve as a key to understanding the structural features of the given sodium modification as a coolant for nuclear power plants with the purpose to decrease its chemical activity in environment and to maintain an automatic clearing of sodium fires.

The neutron diffraction experiment was performed with DIN-2PI time-of-flight spectrometer running from IBR-2 pulsed reactor (Frank Laboratory of Neutron Physics, JINR, Dubna). The neutron momentum transfer, Q, covered in the experiment is comprised $0.3 < Q < 20$ Å^{-1} with resolution estimated as $\Delta Q/Q \sim 5$ %.

Samples of the Na–Pb alloy are made as cylindrical layer of 8 mm in thickness, 30 mm in outer diameter, and 110 mm in height cased in vanadium foil container of 0.15-mm wall thickness to avoid side coherent scattering effects. The measurements were performed on Na–Pb alloys with lead concentration of 7.9 and 3.6 at.%, and pure sodium as reference system at 700 K.

The measurement procedure and primary data processing were standard for such a kind of experiments. The correction on self-shielding the sample in the container, the container itself, standard vanadium sample were introduced. The effect of container scattering was taken into account. The special attention was paid to the multiple scattering correction because it plays a crucial role in the region of small Q for the coherently scattering materials. The corrections on inelastic scattering and recoil effects were introduced.

Static structure factors $S(Q)$ and radial distribution functions of particles $g(r)$ for liquid Na–Pb alloys are obtained. The observed features of the microstructure are discussed.

This work was performed under support of the Russian Foundation for Basic Research, Project № 02-02-17236.

NEUTRON SCATTERING STUDY OF PHASE TRANSFORMATIONS IN SOLID SOLUTIONS $X_{0.25}CU_{1.75}SE$ (X=LI, AG)

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In present work results on the structure studies of solid solutions $Li_{0.25}Cu_{1.75}Se$ and $Ag_{0.25}Cu_{1.75}Se$ are presented. It is established, that in a solid solution $Li_{0.25}Cu_{1.75}Se$ transition to supereionic phase with face centered cubic (fcc) selenium and disordered cation sublattices happens through a number of subsequent phase transitions. With growth of temperature, cation sublattice gradually disorders that results in a modification of overall symmetry. $Ag_{0.25}Cu_{1.75}Se$ is a mixture of phases at room temperature and at $T > 473$ K is a solid solution on the base of fcc lattice.

AVERAGE STRUCTURE IN STOICHIOMETRY DEPENDENT α-$Cu_{2-\delta}Se$

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A structure of the α-phase in copper selenide with different stoichiometric composition, $Cu_{1.78}Se$, $Cu_{1.8}Se$, $Cu_{1.85}Se$ and Cu_2Se, has been analysed by X-ray and neutron diffraction. The high-temperature α-phase of $Cu_{2-\delta}Se$ has $Fm\bar{3}m$ symmetry with copper ions distributed randomly over the interstitial sites within the cubic closed packed selenium sublattice. A tetrahedral environment for copper ions was found in Cu_2Se and $Cu_{1.85}Se$ compounds in contrary to $Cu_{1.78}Se$ and $Cu_{1.8}Se$ compounds where only a small amount of cations in the octahedral interstices have been observed. The lack of octahedral occupation in Cu_2Se and $Cu_{1.85}Se$ can result from larger Cu^+-Cu^+ repulsive interactions for octahedral cations in compounds with a higher copper content.

X-RAY AND NEUTRON DIFFRACTION STUDY OF CRYSTAL STRUCTURE IN $K_{1-x}(NH_4)_xCI$ MIXED SALTS

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The crystal structure of the $K_{1-x}(NH_4)_xCI$ mixed salts with different composition x=0.1, 0.2, 0.5, 0.6, 0.8 has been studied by X-ray and neutron diffraction techniques at room temperature. $K_{0.8}(NH_4)_{0.2}CI$, $K_{0.9}(NH_4)_{0.1}CI$ compounds have $Fm\bar{3}m$ symmetry and $K_{0.2}(NH_4)_{0.8}CI$ compound belongs to $Pm3m$ space group. $K_{0.5}(NH_4)_{0.5}CI$, $K_{0.4}(NH_4)_{0.6}CI$ compounds consist of two phases with space groups $Fm\bar{3}m$ and $Pm3m$. Lattice parameters, positions and thermal parameters of N, K and CI ions have been refined using x-ray diffraction study. Coordinates of hydrogen atoms for $K_{0.8}(NH_4)_{0.2}CI$ and $K_{0.2}(NH_4)_{0.8}CI$ have been determined with neutron diffraction study.

PHONON DENSITY OF STATES IN SUPERIONIC AND NON-SUPERIONIC $LI_{0.25}CU_{1.75}SE$

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Results on the lattice dynamics of the ternary superionic conductor $Li_{0.25}Cu_{1.75}Se$ are presented. The lattice dynamics in $Li_{0.25}Cu_{1.75}Se$ was studied by inelastic neutron scattering over a wide temperature range above and below the temperature of the superionic phase transition. The phonon density of states is analysed together with the crystal structure data.

Diffraction measurements showed that $Li_{0.25}Cu_{1.75}Se$ has a low-symmetry structure similar to the structure of the non-superionic phase of Cu_2Se. The phase transition to superionic phase was determined at about 500±5 K from differential calorimetric analysis (DTA) and temperature dependent X-ray measurements.

Phonon density of states $G(\omega)$ in $Li_{0.25}Cu_{1.75}Se$ was measured at room temperature and 518 K. The phonon density of states at room temperature consists of two parts: the low-energy part at the energy up to 30 meV and the high-energy part at 45-90 meV. At room temperature the low-energy part of $G(\omega)$ in $Li_{0.25}Cu_{1.75}Se$ is similar to the phonon density of states of binary Cu_2Se. Two main peaks at 8 and 21 meV are observed in the low-energy part of $G(\omega)$, which are most probably connected with acoustic and optic vibrations of copper and selenium atoms. The high-energy band in non-superionic $Li_{0.25}Cu_{1.75}Se$ shows two well-defined peaks at the energy range 55–80 meV and could be related to transverse and longitudinal vibrations of light lithium atoms.

In the superionic state a smearing of all phonon modes has been observed. The most pronounced changes occur in the high energy part of G(ω), where „lithium" peaks are broadened drastically and merge with low-energy density of states. The modification of G(ω) at the superionic phase transition is caused by order-disorder transitions and also by effects of anharmonicity at elevated temperature.

INELASTIC NEUTRON SCATTERING STUDY OF INTERCALATED COMPOUND Fe_xTiSe_2

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Materials with polaron charge carriers are at present under close attention because of their unusual properties such as superconductivity, colossal magnetoresistence etc. Theoretical approach for adiabatic single-particle approximation predicts an absence of influence of polaron charge carriers on crystal lattice [1]. However, in dense polaron systems, localization of polarons causes a growth of the density of states at the Fermi level and affects the elastic constants. Earlier, some indirect experimental data about such an influence were obtained as evidence of diffraction line broadening upon localization of polarons [2]; temperature dependence of thermodynamic functions was also possible to describe only if to take into account influence of localization of polarons on lattice elasticity [3]. In this work we present results on inelastic neutron scattering experiment with two differently treated $Fe_{0.25}TiSe_2$samples of; one sample with polaron charge carriers was slowly cooled and another one without polarons was quenched from 800°C, above the temperature of thermal dissociation of polarons). For a comparison the pristine $TiSe_2$ material was also investigated. The measurements have been carried out on spectrometer DIN-2PI, Dubna.

The high frequency edge of the acoustic branch for $TiSe_2$ coincides with Debye temperature T_ϑ determined from heat capacity measurements. Insertion of Fe leads to significant broadening of the phonon lines, which is a result of structural disorder. The difference plot for spectra of slowly cooled (with polarons) and quenched (without polarons) $Fe_{0.25}TiSe_2$ demonstrates an increase of intensity for both low- and high frequency edges of the acoustic branch. We suppose that low-frequency contribution is a result of lattice softening, while the high-frequency one is caused by growth of the T_ϑ for material with polaron localization. This effect may be connected with formation of additional covalent bonds upon localization of polarons [2,3]. So we can conclude, that T_ϑ is not an appropriate parameter for characterization of lattice dynamic for dense polaron systems; influence of polarons on phonon spectra exists for characteristic energy bonds, which are responsible for polarons localization.

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VIBRATION SPECTRA OF Ti-Zr-SI METALLIC GLASS

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The Ti-Zr-Si metallic glass represents a particular system for inelastic neutron scattering (INS) technique. It appears to be possible to select specific concentrations of Ti and Zr in the glassy state which in accordance with Bhatia-Thornton theory will allow for a determination in pseudo-binary approximation the dynamic structure factors S(Q,E) corresponding to only topological short range order $S_{NN}(Q,E)$ ($Ti_{25}Zr_{61}Si_{14}$), chemical short range order $S_{cc}(Q,E)$ ($Ti_{64}Zr_{22}Si_{14}$) or number-concentration $S_{Nc}(Q,E)$ ($Ti_{58}Zr_{28}Si_{14}$). The samples with these compositions, together with the metallic glass $Ti_{86}Si_{14}$ (the latter gives the general dynamic structure factor S(Q,E)) were produced by the melt spinning technique. The measurements have been carried out for the determinations of dynamic structure factors S(Q,E) at temperatures of 300 and 5 K on the IN4 time-of-flight (TOF) spectrometer (ILL, Grenoble), using incident wavelength λ=1.1 Å, and at 300 K on KDSOG TOF spectrometer (JINR, Dubna) for the determinations of S(Q,E) for $Ti_{64}Zr_{22}Si_{14}$ and $Ti_{58}Zr_{28}Si_{14}$ metallic glasses The TOF spectra were converted into generalized phonon density of states G(E), spectra of intensities $I_{NN}(Q)$, $I_{cc}(Q)$, $I_{Nc}(Q)$, I(Q) which are proportional to static structure factors and intensities $I_{NN}(Q,E)$, $I_{cc}(Q,E)$, $I_{Nc}(Q,E)$, I(Q,E) which, calculated without corrections for multi-phonon scattering, are proportional to dynamic structure factors. It is noticed that cooling is accompanied by change in G(E) and I(Q,E) spectra.

THE STUDY OF AMMONIUM ION DYNAMICS IN THE $K_{1-x}(NH_4)_xCl$ MIXED CRYSTALS

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The region of solid solutions near the potassium in dynamic disordered cubic α-phase of the $K_{1-x}(NH_4)_xCl$ mixed crystals is interesting for the study of ammonium ion dynamics. The study of ammonium dynamics in this region at 20 K is carried out with the help of the inelastic incoherent neutron scattering on NERA-PR time-of-flight neutron spectrometer set on pulsed neutron source IBR-2 (JINR, Dubna, Russia). It is shown that at 20 K low energy excitations at 2.4-2.8 and 8.5-9.1 meV are observed only in disordered α-phase and are absent in ordered tetragonal γ-phase near NH_4. The energies of local translational and librational modes are determined also at 20 K in α- and γ-phases.

LATTICE DYNAMICS OF HYDROGENATED AUSTENITIC STEELS

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We investigated the crystal structure and hydrogen vibrations in samples of Fe-18Cr-10Ni and Fe-25Cr-20Ni austenitic steels doped with hydrogen at elevated temperature in a hydrogen gas atmosphere at pressures up to 7 Gpa. Experiments were performed with Filter Analyser Neutron Spectrometer (FANS at NIST) in the Be-graphite-Be mode and with time-of-flight instrument TOSCA at ISIS Facility, RAL.

The previous neutron diffraction experiments [1] show that in the studied steels H occupies the octahedral sites in fcc lattice. Hydrogen-induced martensitic transformations are observed at H/Me>0.4 in Fe-18Cr-10Ni steel. In more stable Fe-25Cr-20Ni steel the volume fraction of ε_H-martensite is less then 5-10% at H contents up to H/Me=0.9. The phase transformation in the both steels starts at higher H contents and fraction of hcp ε_H-phase is lower then in the samples prepared by cathodic charging.

The vibrational energy of H in studied steels decreases from 132 meV at H/Me=0.0033 to 111 meV at H/Me=0.9 reflecting the decrease of the H-Me interaction with increasing lattice parameter. Hydrogen frequency is noticeably higher then in fcc hydrides (except Mn), but much lower then frequency of H in the tetrahedral positions. The vibrational hydrogen peaks are broadened: at H contents from 0.003 to 0.4 - where the single broad peak is observed - the broadening is most probably connected with the Me-H force constant disorder in the present multi-component alloy. At H/Me>0.4-0.5 - where H-peak has the two-component structure - the H-H interaction becomes important resulting in the dispersion of the optical phonon branches. An alternative reason for the splitting of the hydrogen peak could be phase transformations. However it should be probably excluded because our diffraction data show much lower fraction of ε_H-phase then is estimated from the ratio of H-peak components.

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LATTICE DYNAMICS IN AUSTENITIC STAINLESS STEELS

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Inelastic neutron scattering was used to investigate the lattice dynamics in austenitic stainless steels Fe-18Cr-10Ni, Fe-25r-20Ni and Fe-18Cr-16Ni-10Mn. The investigations have been carried out on polycrystalline plates by time-of-flight methods at spectrometer DIN-2PI at JINR, Dubna. The experimental data were corrected for background and detector efficiency. From the scattering function $S(Q,\omega)$ the phonon density of states $g(\omega)$ was obtained. The contribution due to multiphonon scattering was calculated and removed. The data were used to calculate the Debye temperature and specific heat capacity C_V. We also derived the phonon dispersion curves of steels Fe-25Cr-20Ni and Fe-18Cr-16Ni-10Mn by triple-axis spectroscopy.

The phonon density of states calculated from Born-von Karman force constants agrees well with our results obtained by time-of-flight spectroscopy.

DETERMINATION OF THE HYDROGEN CONTENT IN CONSTRUCTIONAL MATERIALS BY SLOW NEUTRON SCATTERING METHODS

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In this work the results of determination of concentration of hydrogen in alloys $ZrNb_{0.01}$ by a method of slow neutrons scattering are submitted. The data of experiments are analyzed with the purpose to establish the possibility of nondestructive controls of the contents of hydrogen in samples of constructional and nuclear reactor materials, in particular, in getter tube of experimental models of fuel element.

The samples of getter tube from an alloy $ZrNb_{0.01}$ being included in a compound of the core of an experimental model of fuel element, as in an initial condition (before tests), so after oxidation of an experimental model in Pb-Bi bath at the temperature of 610°C with during 15-th hours, were investigated. Investigations of blanks of $ZrNb_{0.01}$ alloys for manufacturing of getter's tube and the same samples, but saturated by known quantity of hydrogen from a gas phase, were also executed. In neutron experiments the contents of hydrogen was determined on intensity of incoherent scattering of neutrons in diffraction spectra of the samples. Increase of incoherent background in spectra of samples after oxidation tests were noted. The special measurements of a polyethylene samples were executed with the purpose of calibrations of the results obtained on samples $ZrNb_{0.01}$. By the calibration relations the contents of hydrogen in researched samples were determined. The satisfactory goodness of fit with results of investigations on mass-spectrometer is obtained. The capability and promise of use of scattering of neutrons for nondestructive research of the contents of hydrogen in materials with accuracy of several units wppm is shown.

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THE SMALL ANGLE NEUTRON SCATTERING ON THE EXTENSIVE DEFECTS IN THE PR - SUBSTITUTED $BI_2SR_2CACU_2O_8$

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Phase transformations in high-Tc materials leading to a formation of "superconductor(matrix)/non-superconductive inclusion" composite is a prospective way to improve pinning properties of the materials. Since a cation diffusion in $Bi_2Sr_2CaCu_2O_8$ (Bi-2212) based compounds is quite sluggish at under-melting temperature, phase transformations in Bi-2212 solid solutions can be triggered off by oxidation of aliovalent cations incorporated into such solutions.

The solid solutions $Bi_2Sr_{1.5}Pr_{0.5}CaCu_2O_z$ before and after annealing in air at 700°Ñ for 24 h were investigated by TEM and small angle neutron scattering with using the YuMO setup. The TEM investigations of the specimens after oxidational annealing showed presence of the precipitates with sizes about 10 nm. This precipitates are absent in the specimens before oxidation.

At momentum transfer range $q = 0.006 - 0.1$ A^{-1} the obtained SANS spectra can be described by power function $I = A/q^n$ with n parameter equal to 3.86(2) for specimen before oxidation and 3.85(5) for oxidated one. From this it can draw the conclusion about the realization of Porod law for scattering on these specimens. From value of the A parameter it can estimate the specific surface area of the specimens. This area is 9.4(8) m^2/cm^3 for the specimen before oxidation. At probable assumption about the lamellar structure of investigated material this surface area value corresponds to thickness of lamellas about 68 nm. This result can believe that the main contribution to scattering in both samples put the stacking faults, which present usually in compounds with $Bi_2Sr_2CaCu_2O_8$ structure.

The difference of the SANS spectrum for the specimens after and before oxidation at range $q = 0.006 - 0.1$ A^{-1} is described by the same power function with parameter $n = 3.5(2)$. This value of parameter corresponds to polydisperse precipitates or to the fractal scattering surface. The intensity of scattering on the staking faults is about 1000 cm^{-1} and the intensity of scattering on the precipitates is about 10 cm^{-1}. Therefore the exact calculation of the specific surface area of precipitates is impossible. The estimation of this area from the difference of the specific surface area of the specimens after and before oxidation gives the value about 1.5 m^2/cm^3.

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SELF-ASSEMBLY OF POLYELECTROLYTE RODS IN POLYMER GEL AND IN SOLUTION: SMALL-ANGLE NEUTRON SCATTERING STUDY

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The aggregation of rigid-rod polyelectrolyte based on poly(sodium p-phenylenesulfonate) was studied by small-angle neutron scattering in aqueous solution and inside water-swollen polyacrylamide gel. It was shown that both inside the hydrogel and in solution polyelectrolyte rods self-assemble into cylindrical aggregates with the polymer chains being aligned parallel to the axis of the aggregate. The radial aggregation number of these aggregates was calculated to be about 8-9 single polymer chains in the cross-section of the aggregate. The length of these aggregates is much higher than the contour length of a single chain. Gels with embedded rods were studied by contrast variation method in order to examine separately the scattering by the gel and by the rods. Two important observations were made. First, it was shown that the ordering of the rods in the gel resembles that in solution. Second, it was shown that the gel itself is more homogeneous in the presence of rods. The last effect may be attributed to the presence of the mobile counterions of the rods, which counteract the formation of spatial inhomogeneities in the network during synthesis, because the inhomogeneous distribution of the network mobile counterions should be also accompanied by the inhomogeneous distribution of the mobile counterions of the rods, that is associated with significant translational entropy losses.

SANS and SAXD STUDY OF DNA+DOPC+Ca^{2+} AGGREGATES

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DNA aggregates with neutral phospholipids formed in aqueous phase in the presence of metal or amphiphile cations can be used as nonviral vectors for transfer and expression of DNA in cells. Small angle neutron scattering (SANS) and small angle x-ray diffraction (SAXD) methods were used for the study of the structure aggregates of DNA and dioleoylphosphatidyl-choline (DOPC) liposomes in presence Ca^{2+} ions.

Unilamellar liposomes were prepared by extrusion of DOPC multilamellar dispersion in presence of 20mmol/l $CaCl_2$ through polycarbonate filter with 50nm pores. High polymerized DNA from calf thymus and DNA fragments of approx. 500bp length were used for the creation of aggregates at DNA:DOPC=1:2 and 1:10 base/mol in 20mmol/l $CaCl_2$. The SANS measurements were performed at the small-angle time-of-flight axially symmetric neutron scattering spectrometer YuMO at the IBR-2 fast pulsed reactor of the Frank Laboratory of Neutron Physics, JINR in Dubna. The samples were measured in quartz cells of 1 mm thickness at 25.0±0.1°C. The dependence of SANS intensity $I(q)$ on the scattering vector $q=4\pi\sin\theta/\lambda$, where 2θ is the scattering angle, have shown the presence of Bragg peak (Fig.1). We have observed the changes in the intensity of peak in dependence on the molar ratio of DNA:DOPC in the sample. Multilamellar DOPC dispersion in the presence of 20 mmol/l $CaCl_2$ was used for the creation of DNA:DOPC aggregates at different molar ratio for SAXD experiments. Synchrotron radiation x-ray diffraction measurements were performed at the A2 soft-condensed matter beam line at HASYLAB at the Deutsches Elektronen Synchrotron (DESY) in Hamburg, using monochromatic radiation of λ=0.15 nm wavelength. The samples were measured at 20°C.

Data reduction and normalization were done with the programs STAFO and OTOKO.

The dependencies of SAXD intensity $I(s)$ on the reciprocal spacing $s=q/2\pi$ have shown 4-5 reflexions, which were analysed as superposition of two one- dimensional phases. The intensities of reflections (but not their positions) changed in dependence on the molar ratio of DNA:DOPC. The repeat periods d_1=7.41±0.03 nm and d_2=5.97±0.01 nm are indicated in Fig.1 by vertical lines.

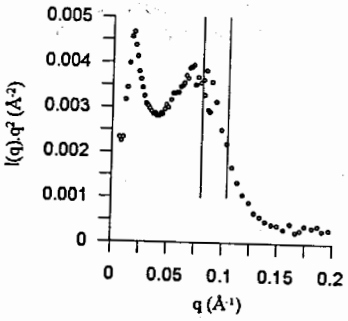

Fig.1. The dependence of SANS intensity on q of DNA:DOPC=1:2 base/mol in 20mM $CaCl_2$.

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EFFECT OF CHOLESTEROL ON THE BILAYER THICKNESS IN UNILAMELLAR EXTRUDED DLPC AND DOPC VESICLES

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Cholesterol in the bilayer of model and biological membranes affects protein sorting and translocation, protein conformation and lateral aggregation. These effects can be caused by lipid bilayer thickness changes induced by cholesterol. In the present contribution, small-angle neutron scattering (SANS) on extruded (500 Å) unilamellar vesicles was used to study lipid bilayer thickness when cholesterol (CHOL) was added at 0.8 molar ratio to DLPC (1,2-dilauroylphosphatidylcholine) or DOPC (1,2-dioleoylphosphatidylcholine) bilayers. The SANS curves were measured on YuMO spectrometer at 3 different contrasts (at volume fractions of H_2O in D_2O x_w=0, 0.3 and 0.5) and 30°C when the bilayers are in the condensed fluid state. The SANS data were evaluated supposing that the SANS on vesicles dispersed in the aqueous phase can be approximated in the range of scattering vector values q corresponding to interval 0.001 $Å^{-2} < q^2 < 0.006$ $Å^{-2}$ by scattering on randomly oriented planar bilayers. Using the small–angle form of Kratky-Porod approximation $I(q)\sim q^2\exp[R_g^2(x_W)q^2]$ of the normalized SANS intensity $I(q)$, the bilayer gyration radius R_g taken perpendicularly to the bilayer and the intercept $\lim I(q)q^2$ at $q\to 0$ were obtained at each x_w. From the linear dependence of $[\lim I(q)q^2]^{0.5}$ on x_w, the average scattering length density of the lipid bilayer ρ_L was calculated from the match point $x_{w,m}$ at which $[\lim I(q)q^2]^{0.5}=0$. Using the linear dependence of $R_g^2(x_W)=R_{g,\infty}^2+\alpha\Delta\rho^{-1}$ (where $\Delta\rho=[\rho_L-\rho_w(x_w)]$ is the value of contrast and $\rho_w(x_w)$ the average scattering length density of the aqueous phase at x_w), the gyration radius at infinite contrast $R_{g,\infty}$ and the parameter α were obtained. The value of $d_g=12^{0.5}R_{g,\infty}$ characterizes the bilayer thickness, and α is a measure of the scattering length density difference between the bilayer polar and hydrophobic regions. It is seen from the values obtained (Table) that cholesterol increases the thickness d_g in DLPC vesicles, while in DOPC vesicles the value of d_g is not affected within the experimental error. Similarly, the parameter α is increased in DLPC vesicles due to the presence of cholesterol but not in the DOPC vesicles. The polar region thickness in PC bilayers is d_P=9.0±1.2 Å, the hydrophobic region thickness in the DLPC monolayer is thus $d_C=(d_g-2d_P)/2$=11.94±1.31 Å, while in the DOPC monolayer d_C=13.79±1.38 Å. The long axis dimension of cholesterol monohydrate molecule is 17 Å. The observed larger change in the DLPC bilayer thickness can be thus explained by the larger hydrophobic mismatch of cholesterol molecules with the DLPC hydrocarbon region in comparison to DOPC. The bilayer thickness changes induced by cholesterol via the hydrophobic mismatch can be important for the regulation of membrane functions.

Vesicles	d_g (Å)	10000α
DLPC	41.87±1.04	1.21±0.24
DLPC+CHOL	46.16±0.21	1.91±0.16
DOPC	45.58±1.38	1.67±0.36
DOPC+CHOL	46.34±1.14	2.08±0.30

This work was supported by the JINR project 07-4-1031-99/03 and by the VEGA grant 1/0123/03.

STRUCTURAL CHANGES IN MITOCHONDRIA STUDIED BY SMALL ANGLE NEUTRON SCATTERING

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It is known that swelling of mitochondria in hypotonic media simulates qualitative changes the kinetic properties of the system of respiration and oxidative phosphorylation. In present work the structure of intact mitochondria from rat liver were studied by SANS. Mitochondria were incubated in media with different tonicity from 300 to 120 mosM. It was noticed that the curves from mitochondria imbedded in various media were differed each other. In particular, the diffuse maximum was observed under hypotonic conditions. This maximum centered near scattering vector 0.04 $Å^{-1}$ that conform to objects with size about 150 – 190 Å. Also one examined of influence of temperature on change in structure of mitochondria in respective media. Besides the contrast variation was realized.

STUDY OF MICELLAR SOLUTIONS USED FOR ETCHING OF NANOPORES IN POLYMERS

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Study of micellar structure of surfactant solutions is of great interest in connection with the recently revealed phenomenon of the surfactant-controlled etching of ion track nanopores [1-3]. In experiments on ion-irradiated polymers it was shown that etching in alkaline solution containing small amounts of surfactants is strongly influenced by surfactant molecules that adsorb on the polymer surface and change susceptibility of the surface to chemical attack. The adsorbed surfactant layer is, in fact, a self-assembling system created on the polymer surface and in narrow pores. The surfactant molecules form micelle-like aggregates at the entries of nanopores, which prevent further penetration of surfactant into the growing pore channel. This opens the way to control the nanopore size and shape by the choice of a surfactant with appropriate properties. The method can be applied to the production of high-performance ultrafiltration membranes and various nanoporous materials. In order to better understand the mechanism of the phenomenon it is essential to measure characteristics of electrolyte solutions containing the surfactant. First of all, it is important to know the critical micelle concentration and the micelles' size and shape in the solutions used for etching (water + alkali + surfactant) and in the model solutions (water + neutral electrolyte + surfactant).

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STUDY BY SANS METHOD THE INFLUENCES OF O-p-NITROPHENYL-O,O-DIMETHYLTIOPHOSPHATE UPON THE POLYMER-COLLOIDAL COMPLEXES

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In this report we show the results of lasting studies of influence polymer - polyethylenimine (PEI), as well as phosphorus substrates upon the geometric features of cetyltrimethylammonium bromide (CTAB). Earlier we studied geometric features of colloidal particles, formed by PEI with MM 30000 and CTAB in the water media. It is very interesting to investigate the influence of polymer chain length on geometric and catalytic in respect of decompositions a substrate O-n-nitrophenyl-O,O-dimethyltiophosohate properties of systems. For this we used PEI with MM 1200.

There is a different chemical behavior of the substrates in the system CTAB-PEI (1200)-water. It was shown from results of UV-spectral analysis. We may see the offset of the substrate absorbing band and the increasing its intensity to account of forming a molecular complex CTAB-PEI (1200)-substrate up to C_{CTAB} = CCM (critical micelle concentration). We observed in greater degrees an attack at the atom of carbon from methyl group, and at the atom of phosphorus to a lesser extent after the C_{CTAB} > CCM. We have used the SANS method and have shown strong decreasing of intensity of scattering of neutrons, being indicative of reducing the micelles concentrations at introduction to system PEI. This effect is stronger at the high concentration of polymer. It is possible as a result of sitting of micelles to polymeric chain. The neutron scattering curves have a maximum for concentrations PEI 0.02M and 0.2M and this indicates about the interaction of associates and about the structuring of media of reaction proceeding. Under the greater concentrations (0.6M) maximum is absent, obviously as a result screening charged micelles by the polymer.

RESEARCH OF CdSe LUMINESCENCE NANOCRYSTALS WITH USE OF SUBMICRONIC CONFOCAL RAMAN MICROSCOPE

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It is presented the description of confocal Raman microscope, its optical circuit and characteristics. The first results are submitted on measurement of spectra of luminescence of CdSe clusters, synthesized in reaction between acetate of cadmium and selenourea in pyridine.

The average size of clusters, measured by a method of small-angle scattering of x-ray, is 1,6÷1,8 nanometer. Clusters CdSe are put on optically transparent microspheres in the size about 1 micron.

Spectra of luminescence of CdSe clusters are resulted at excitation by the laser with length of a wave λ_0=441,8 nanometer. The Raman mode are presented with corresponding to structure of CdSe crystals. The spectral resolution of Raman mode is $\Delta r \approx 10 sm^{-1}$.

The structure of microsphere with taking place on a surface CdSe clusters in luminescent light has been measured in the mode 3-D scannings.

STRUCTURE AND LATTICE DYNAMICS IN RELAXOR PLZT X/65/35 CERAMICS IRRADIATED BY HIGH-CURRENT PULSED ELECTRON BEAM

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Recently we have found [1] that influence of high-current pulsed electron irradiation with energy E=250 keV on the structure and lattice dynamics transformation of relaxor PLZT ceramics related with the charge storage in lattice which leads obviously to the change of ion charge, redistribution of vacancies in A and B sublattice [2].

In this paper we present the structure refinement of similar PLZT 8/65/35 ceramics (space group R3m, Z=1) before and after irradiation by high-current pulsed electron beam with energy E=800 keV using X-ray diffraction investigations. The lattice dynamics is performed by IR and Raman spectroscopy studies in the spectral range 50–2000 cm^{-1}. Optical spectra in the range 325–1000 nm shown the behavior of the fundamental absorption edge. The obtained results reveal the splitting of several X-ray diffraction peaks associated obviously with the appearance of a new phase. Besides, both the increase of intensity and shift TO2, TO3 and TO4 Raman's active modes towards the lower wavenumber region related obviously with the heat annealing of irradiated sample.

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NEUTRON PHYSICS STUDIES OF FUNDAMENTAL PROCESSES IN CONDENSED MEDIA

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A review of experimental and theoretical investigations of 1) dipole-dipole incoherent delocalization of excitations and 2) multiple small angle scattering of waves in statically disordered media is presented. Main attention is devoted to systems wich can be studied by methods of neutron physics.

The delocalization of excitation is studied on the example of depolarization of beta-active nuclei 8Li in statically disordered impurity system 8Li-6Li in single crystal LiF. Theoretical problems related with microscopical derivation of corresponding master equations and long time asymptotics of its solution averaged over random impurity distribution are described. Detail discussion of experimental studies of the process by beta-NMR specrtoscopy is presented.

Discussion of the multiple neutron scattering includes: Moliere-Bethe theory, double-crystal diffractometers, dependence of the width of the scattering cross-section on the density of scattering grains and new general theory, which describes multiple neutron scattering, taking into account pair correlations in grains positions.

Session
“Neutron Physics”

NUCLEAR DATA REQUIREMENTS FOR THE ACTINIDES AND FISSION PRODUCTS BUILD-UP AND BURN-UP

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Fast pulse reactors exhibit high neutron fluxes, and represent major facilities in which important nuclear cross-section measurements can be conveniently undertaken for the study of the build-up and burn-up of actinides. More accurate nuclear data are also required for inventory calculations of the most important fission products contributing to the reactor kinetics as well as in decay heat and long-lived fission product radiotoxicity studies.

The present status of the nuclear cross-section data is discussed with respect to the build-up and burn-up of the nuclides in the reactors. Specific needs are identified, along with the data requirements of those long-lived radionuclides that contribute significantly to the long-term activity of spent fuel. To do this, the inventory of actinides (from ^{234}U to ^{244}Cm), long-lived fission products (^{79}Se, ^{85}Kr, ^{90}Sr, ^{93}Zr, ^{93m}Nb, ^{99}Tc, ^{107}Pd, ^{126}Sn, ^{129}I, ^{135}Cs, ^{137}Cs, ^{147}Pm and ^{151}Sm) and fission products determining the criticality in realistic thermal reactor burn-up calculations were analysed. The experimental data, the results of different burn-up calculations for fission products and cumulative yields without burn-up were compared. A large difference between two shows the importance of some neutron reaction cross sections for these nuclides in inventory calculations. The spread of data for the first two characterizes the uncertainty with which we know the cross sections and decay data.

The quality of cross sections determining the build-up and burn-up of nuclides, important for the criticality and nuclear waste management of thermal reactors was reviewed; a list of cross sections needing improvement was prepared. Requirements for new measurements of some cross sections important for the development of advanced systems with closed fuel cycle and full actinide recycling were considered in few of the present knowledge of these cross sections.

QUANTIFICATION OF DATA UNCERTAINTIES

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Covariance matrices are widely used to quantify the uncertainties of evaluated data obtained by a model or non-model least squares fit of the experimental data. Greater accuracy can be achieved through this approach if the experimentalists publish detailed descriptions of the raw data reduction procedure, corrections introduced and error components assigned including their correlative properties. Correlations with other data measured at this installation or due to the use of the same sample, detector, etc. should be noted. The covariance matrix of uncertainty of experimental data, prepared in the case of incomplete information about the experiment, can lead to the bias in the evaluated values, even when data look consistent.

Highest requirements to the quality of the data should be applied to the neutron cross-section evaluations for reaction standards. Last (1991) evaluation of the standards was based on R-matrix model least squares fit for light nuclei and non-model fit for heavy nuclei. The strong reduction of uncertainties observed in the model fit was considered as unrealistic one, and experts substantially increased the final recommended uncertainties. To study the reasons of this reduction, the IAEA organized the Co-ordinated Research Project (CRP) on the Improvement of the Standard Cross Sections for Light Elements. The first results obtained in the CRP were presented at the First Research Co-ordination Meeting [1] and are summarized in this paper together with the author's contributions and post-meeting discussions.

It is shown that the central values and covariance matrix of uncertainty of evaluated data obtained with the non-model Bayesian code GLUCS and the general least squares code GMA agree with the limits of numerical inaccuracy explained by the use of different equations. A special test is demonstrated that the results of the evaluation are reliable and numerically stable even when very many sets of correlated data are fitted. It is proposed a collapsed one-group variance as simple and convenient measure for characterizing the data uncertainty, a measure which practically does not depend on the model function used in the fitting, or if it is a non-model fitting at all. The physical reasons leading to the reduction of evaluated data uncertainty are discussed. The effect of bias of evaluated data, known in the nuclear data community as Peelle's Pertinent Puzzle, is discussed for a realistic case of fitting of the experimental data, and technical recipes to reduce it are considered. It is shown that the best estimation of the unbiased true value and physically justified covariance matrices of uncertainties for the evaluated standard reactions cross sections can be obtained.

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SEARCH FOR RADIATIVE BETA-DECAY OF THE FREE NEUTRON

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We conducted the experiment on radiative neutron beta-decay on a intensive cold neutron beam at ILL during April and May of 2002 [1]. Results of this first experimental search for the radiative decay mode of the free neutron are reported. The gamma-spectrum was studied in the region from 35 keV to 100 keV. Whereas the radiative decay mode could not actually be established, the statistics collected allow one to deduce an upper limit of 6.9×10^{-3} (90 % C.L.) for its branching ratio in this energy region. This value is only a few times grater, than the theoretical prediction based on the standard model of weak interactions. This fact, in turn, means that we have come very close to discovering the radiative neutron decay mode.

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ABOUT STABILITY OF A GAMMA-REGISTRATIONS FOR Ge(Li)-DETECTORS AT LONG TIME INTENSIVE RADIATION

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Session "Neutron Activation Analysis for Life Sciences"

NEUTRON ACTIVATION ANALYSIS OF MERCURY IN *Spirulina Platensis* USED AS A SORBENT

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The epithermal neutron activation analysis (ENAA) was used for the investigation of interaction blue-green microalga *Spirulina platensis* (*Sp. Pl.*) with mercury. Accumulation of vitally essential elements (Se, I, Cr) by *Spirulina* biomass was investigated and described in previous work performed at the Frank Laboratory of Neutron Physics, JINR and at the E.L. Andronicashvili Institute of Physics of the Georgian Academy of Sciences. The results of the dynamics of absorbtion Hg by *Spirulina* biomass in nutrient medium, accumulation degree of Hg by *Sp. Pl.* during 1-6 days as well as growth of Spirulina biomass are reported. It was shown that *Spirulina* biomass could accumulate toxic element that is of great scientific and practical interest.

HEAVY METAL AND RARE EARTH ELEMENTS DISTRIBUTION IN THE DIFFERENT COMPONENTS OF RYBINSK RESERVOIR ECOSYSTEM

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Nuclear analytical technique – instrumental neutron activation analysis was used to study different components of the Rybinsk Reservoir ecosystem affected by the largest steel-producing metallurgical complex in Europe in the town of Cherepovets.. The Cherepovets metallurgical complex is situated 700 km to the north of Moscow, on the north-east bank of the Rybinsk Reservoir, one of the sources of fresh water to the capital of Russia, Moscow. The reservoir is also plays a very important role in commercial and game fishing. To study migration, accumulation and distribution of the inorganic pollutants within the reservoir ecosystem compartments, 9 sediment samples,10 mollusk samples (shells and mantles), 48 samples of muscles and liver from different species of fish were analyzed. Samples were collected in summer 2001 from 16 sampling sites with different environmental situations and the potential contamination degrees. A total of 45 elements, including most of heavy metals and rare earths, were determined using activation with epithermal neutrons at the IBR-2 reactor in Dubna. The results obtained contribute to understanding of biogeochemistry of element–pollutants in freshwater man-made lake ecosystem. Concentrations of many elements have been found to be higher at locations close to the Volga River channel, *i.e.* quite far away from the Cherepovets industrial center. This may reflect the specificity of Cherepovets industry where, so called «full-cycle steel production» is run. In terms of issues related to the environmental pollution, this means, first of all, the prevalence of pollutants originated from coal processing for producing coke. These are: the polycyclic aromatic hydrocarbons, phenols, organic acids, etc. (Kozlovskaya et al., 1990; Siddall et al., 1994). We presume that influence of these pollutants may have change the regularities of uptake and excretion of elements by biota, *i.e.* the organic pollutants considerably modified ecosystem bio-hydro-chemical regimen in respect to metal and rare earths cycles in it.

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DIRECT MEASUREMENT OF THE NEUTRON-NEUTRON SCATTERING AMPLITUDE AT PULSED REACTOR YAGUAR: CURRENT STATUS OF THE EXPERIMENT

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Knowledge of the neutron-neutron scattering amplitude a_{nn} for thermal neutrons at high precision gives one the possibility to resolve the problem of possible charge symmetry breaking (CSB). For proton-proton interaction corresponding value a_{pp} is well known: $a_{pp} = -17.3 \pm 0.005(stat) \pm 0.4(syst) fm$ [1]. For a_{nn} situation looks more complicated: at the end of 1990's several experiments on indirect a_{nn} measurements gave the value $a_{nn} = -18.7 \pm 0.3(stat) \pm 0.6(syst) fm$ [2-3], which shows that nn- interaction is slightly stronger with $\Delta a_{CSB} = a_{pp} - a_{nn} = 1.4 \pm 0.6 fm$. However recently the situation again changed due to the new experiment on a_{nn} measurements resulting at $a_{nn} = -16.27 \pm 0.4 fm$ [4]. Easy to see that new result gives not only another value of Δa_{CSB}, but also changes it's sign. So, experimental situation requires direct measurements of the a_{nn} value wit accuracy not worse than 2-3%.

The reactor YAGUAR (VNIITF, Snezhinsk, Russia) [5] provides the best conditions presently available for the nn-experiment as suggested in. It has:

- A high, at the level of 10^{18} cm $^{-2}$s $^{-1}$, peak thermal neutron flux density.
- A through-channel in active core with a cylindrical symmetry of the neutron field that should make the experimental data treatment straightforward.
- A possibility of placing the neutron moderator inside the channel
- A relatively short power pulse allowing the use of time-of-flight technique for the separation of thermal neutrons from fast neutrons.

To use all advantages of this reactor effectively, the collaboration for a_{nn} study named DIANNA (Direct Investigation of A_{NN} Alliance) was created. It combines efforts of neutron physics scientists from JINR, the experts from VNIITF with a vast experience in pulsed reactors (the YAGUAR including) design and operation, and the nuclear few body experts from TUNL, ADNA and Gettysburg College with the experience in measuring the a_{nn} amplitude.

Current status of the experiment on direct a_{nn} measurements, proposed by DIANNA collaboration, will be reported.

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