FRANK LABORATORY OF NEUTRON PHYSICS
JOINT INSTITUTE FOR NUCLEAR RESEARCH

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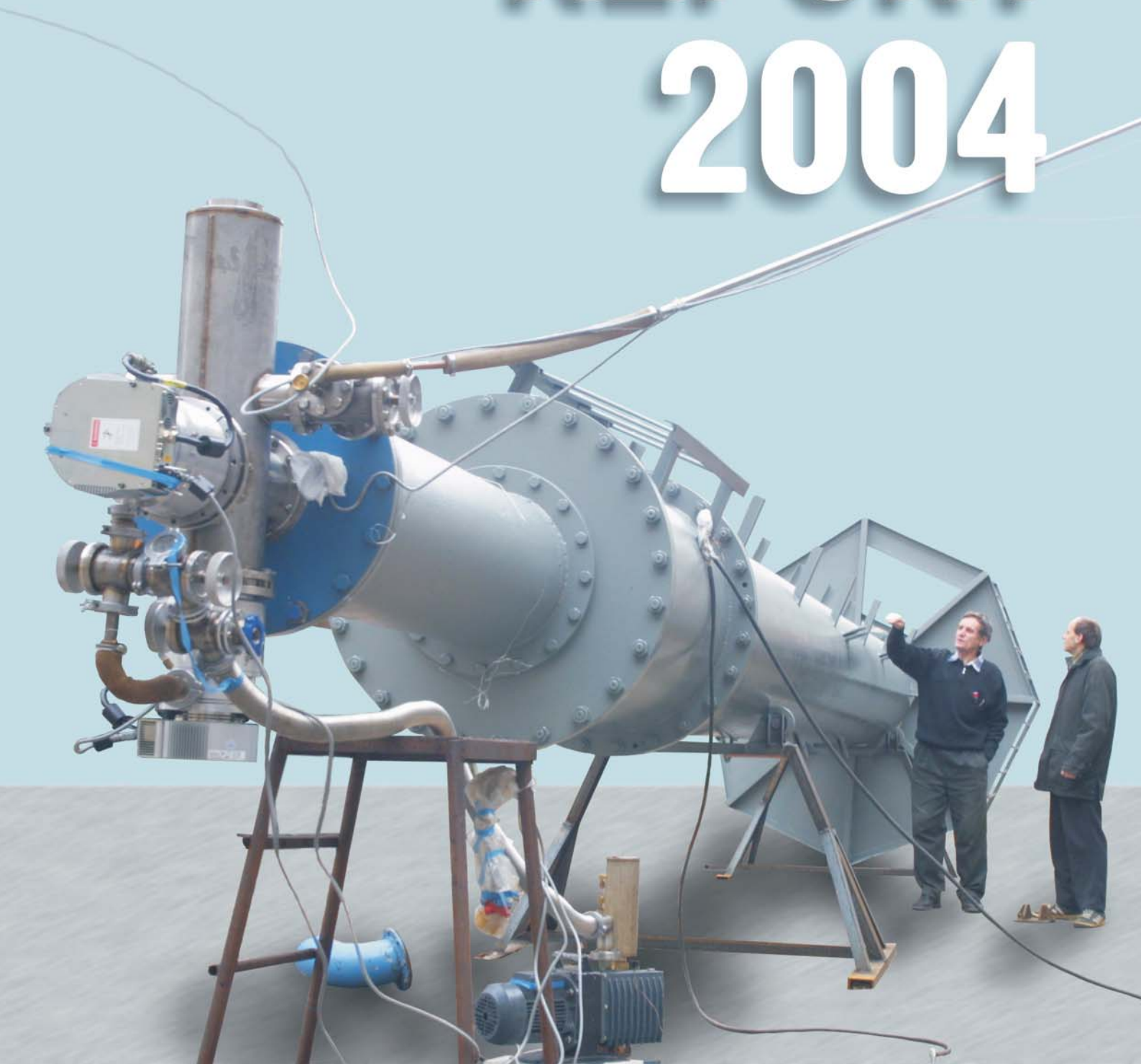

Cover illustration
Vacuum over-reactor channel to investigate the direct measurement of the nn-scattering length at the pulsed reactor JAGUAR (Snezhinsk)

Contacts: FRANK LABORATORY OF NEUTRON PHYSICS
JOINT INSTITUTE FOR NUCLEAR RESEARCH
141980 Dubna, Moscow region, Russia
Fax: (+7)09621-65085
E-mail: khitrov@nf.jinr.ru
http:/nfdfn.jinr.ru/

Editors: A.V.Belushkin, V.A.Khitrov

Translated from Russian: T.V.Avdeeva, E.V.Lokhmatova

Typesetting: V.S.Rumyantseva

Cover: Yu.I.Emelina

Photography: Yu.A.Tumanov

FRANK LABORATORY OF NEUTRON PHYSICS OF THE JOINT INSTITUTE FOR NUCLEAR RESEARCH

The Joint Institute for Nuclear Research (JINR) is an international centre for experimental and theoretical investigations in the fields of elementary particle physics, nuclear and neutron physics, condensed matter research and related topics.

The JINR structure is determined by the fact that it is governed internationally and has many research specializations. Current scientific and financial affairs of the Institute's Laboratories, common services as well as the work of specialized departments are guided by the Institute Directorate.

The Frank Laboratory of Neutron Physics is one of the eight JINR Laboratories. It was established in 1956, soon after the foundation of JINR.

In 1960 a principally new source of neutrons - the IBR fast pulsed reactor of periodic operation - was created at FLNP under the leadership of Prof. D.I.Blokhintsev (11.01.1908 - 24.01.1979). The birth of this reactor gave rise to a new direction in the development of research neutron sources.

An extended scientific program with this reactor was initiated under the leadership of Nobel Prize Winner and Laboratory Director Prof. I.M.Frank (23.10.1908 - 22.06.1990) and Deputy Director Prof. F.L.Shapiro (06.04.1915 - 30.01.1973). Since 1960, a whole family of unique pulsed neutron sources for nuclear physics and condensed matter physics has been developed and constructed. The latest in the family, the IBR-2 high flux pulsed reactor, was commissioned in February 1984. The Laboratory was named after Prof. I.M.Frank in 1992. In the same year, in JINR the I.M.Frank Prize for Neutron Physics was established.

At present, the scientific activity of the Laboratory focuses on two fields of physics, namely nuclear physics and condensed matter physics. The first involves investigations of the neutron as an elementary particle and studies of compound states in neutron induced reactions. The second investigates pressing problems in the physics and chemistry of solid states, surfaces and liquids, and in molecular biology. Applied investigations are also carried out using nuclear physics methods.

PREFACE

We would like to introduce the report on the scientific activity of the Frank Laboratory of Neutron Physics for 2004. The first part is a brief review of the experimental and theoretical results of investigations achieved in the main scientific directions – condensed matter physics, neutron nuclear physics and applied research. The second part includes reports on the operation of the IBR-2 pulsed reactor and realization of the IREN project. The third part is development and creation of elements of neutron spectrometers for condensed matter investigations. The fourth part presents the investigations that characterize the main directions of research in greater detail. The report completes with the list of publications for 2004.

In 2004 the construction of a new movable reflector MR-3 for the IBR-2 reactor was completed. After the assembling and test-bench trials the MR-3 was moved into the reactor building, the MR-3 assembling was carried out at the regular place near the reactor. After testing at the regular place MR-3 was approved to be put into service by GOSATOMNADZOR. From 16.06.2004 to 20.07.2004 the Program to start and investigate the reactor with a new MR-3 was performed. The obtained results are close to the calculated ones. On 20.07.2004 the reactor was put into operation at power 1.5 MWt in the mode of 5 Hz. Thus, a very important stage of the IBR-2 modernization was completed. In September, 2004, the IBR-2 resumed operation for physical experiment: as of 01.12.2004, it operated 4 cycles for physical experiments (≈1400 hours), as planned.

The construction of a new neutron source IREN continued: manufacturing of the main equipment for the electron accelerator LUE-200 was practically completed. However, the lack of financing led to a delay in the completion of mounting and startup of the first stage of the linac (with one klystron for the energy 100 MeV). Technical preparation for dismantling of the IBR-30 reactor completed. The works are to be started in spring, 2005, after receiving the license for putting into operation of the built storage of radioactive elements. Fuel for the IREN multiplying target has been delivered, which makes it possible to start preparation for its manufacturing. But on the whole, due to constant lack of financing of the project, the startup of the first stage IREN facility may be expected no sooner than in 2008.

On the neutron spectrometers of the IBR-2 reactor several interesting experiments were carried out. The obtained results are of principal character. In particular, on the REMUR polarized neutron reflectometer, for the first time, the phenomenon of coexisting of superconductivity and magnetism on the interface in thin layers of a superconductor ($V/Fe_{0.66}V_{0.34}$) and a ferromagnet (Fe/V plus bilayers V/Fe) has been studied. The effect of superconductivity on magnetism has been revealed, which is dependent strongly on the composition and structure of the magnetic layer. On the YuMO small-angle neutron scattering setup a structure of polycarbosilane dendrimers has been

determined. Peculiarities of stacking of end groups of dendrimers, namely their layered character, have been discovered, which may account for a restraint in the growth of dendrimers with increasing generation degree.

In the course of the year a number of works was carried out and some interesting results in the field of nuclear physics were obtained: analysis of the data obtained in the experiments conducted in 2002 – 2003 to search for the negative neutron p-resonance in lead isotopes was completed; at the EG-5 generator of FLNP JINR experiments to measure the energy dependence of the angular distribution coefficients in the reaction $^{14}N(n,p)^{14}C$ for the neutron energy interval ~ 10 keV - ~ 1 MeV started; the measurements under the program for collaboration nTOF – investigations of the nature of vibrational resonances in neutron-induced fission and obtaining of fission cross section data for the solution of ADS-system-related and nuclear waste burning problems, were completed. On the beam PF1 of the reactor in ILL (Grenoble) an experiment to investigate mass-energy correlations in the neutron-induced triple fission was conducted. In the framework of the plan of the preparation of direct measurements of the nn-scattering length at the pulsed reactor JAGUAR (Snezhinsk) the fluxes of fast, epithermal and thermal neutrons over the total depth (~ 12 m) of the under-reactor well were measured. At the reactor in ILL (Grenoble) a UCN storage experiment was conducted. As a result, the existence of an anomalous UCN leakage channel from vessels with perfect walls made from monocrystalline sapphire was demonstrated over a wide temperature range (70-800 K). The new experiment of UCN time focusing was performed. The problem of completely model-absent determination of the density of levels in a fixed interval of their spins and radiative strength functions of dipole electric and magnetic gamma-transitions at excitation energies around the neutron binding energy was solved.

The investigation of the energy quantization effect at the UCN diffraction on the moving grating continued. As was shown earlier, the grating, moving across the direction of the neutron wave propagation, modulates the propagated wave in phase and (or) in amplitude and acts as a non-stationary quantum device. This phenomenon was demonstrated in the experiment carried out at the reactor in ILL (Grenoble). The obtained results are in good agreement with the quantum-mechanical calculation. The phenomenon of neutron energy change at non-stationary influence on the neutron wave opens new experimental possibilities, in particular, a possibility of neutron focusing in time by means of controlled change of their velocity. In recent experiment the efficiency of such time lens was demonstrated. A focusing efficiency is approximately 30% and in future may be considerably increased.

The work to study atmospheric deposition of heavy metals by means of biomonitoring, NAA and GIS technologies (REGATA Project) over the territory of Russia and some other countries continued. Organizational and methodological work to get ready for the next European

simultaneous collection of moss-biomonitors of heavy metal atmospheric deposition (moss-survey) is to be held in 2005 in a number of JINR member and non-member.

A comparative analysis of various biomonitors (lichens, tree bark) and of soils from the region of the oil-refining plant in Constance, Romania, was carried out. Neutron activation analysis of over 250 samples of vegetation and animal origin was conducted under the Coordination Program (2002-2005) and the Project for Technical Cooperation with IAEA (2003-2005) for supervision and quality of food products grown in the conditions of strong antropogenic pollution. The final stage of work under the project «Monitoring of working places and occupational health of personnel engaged in production of phosphate fertilizers» at plants in Russia and other countries (European Program 5, Copernicus) was completed. Work to develop new pharmaceuticals and sorbents on the basis of the blue-green alga *Spirulina platensis* in cooperation with a group of biophysicists in the Institute of Physics of the Georgian Academy of Sciences continued.

The Frank Laboratory of Neutron Physics continues to be one of the leading neutron centers of Europe and develops in spite of all the difficulties connected with severely limited funding.

A.V. Belushkin

Director

9 March 2005

ПРЕДИСЛОВИЕ

Вашему вниманию предлагается отчёт о научной деятельности Лаборатории нейтронной физики им. И.М. Франка за 2004 год. В первой части представлен краткий обзор экспериментальных и теоретических результатов исследований, достигнутых по основным научным направлениям – физике конденсированных сред, нейтронной ядерной физике и прикладным исследованиям. Вторая часть включает отчёты о работе импульсного реактора ИБР-2 и реализации проекта ИРЕН. Третья часть посвящена разработке и созданию элементов нейтронных спектрометров для исследований конденсированных сред. В четвёртой части представлены экспериментальные отчеты, которые более подробно освещают основные направления исследований. Завершает отчёт список публикаций за 2004 год.

В 2004 г. была завершена работа по созданию нового подвижного отражателя ПО-3 для реактора ИБР-2. После сборки ПО-3 и стендовых испытаний он был перевезен в здание реактора, выполнен монтаж ПО-3 на штатном месте около реактора. После испытаний на рабочем месте получено удостоверение ГОСАТОМНАДЗОРА по приемке ПО-3. В период с 16.06.2004 г. по 20.07.2004 г. была выполнена программа по пуску и исследованиям реактора с новым ПО-3. Полученные результаты близки к расчетным. 20.07.2004 г. реактор был выведен на мощность 1,5 МВт в режиме 5 Гц. Таким образом, был завершен очень важный этап модернизации ИБР-2. В сентябре 2004 г. ИБР-2 возобновил работу на физический эксперимент: на 01.12.2004 г. отработал на физические эксперименты 4 цикла (около 1400 часов в полном соответствии с планом.

Продолжались работы по созданию нового источника нейтронов ИРЕН: практически завершено изготовление основного оборудования ускорителя электронов ЛУЭ-200. Однако завершение монтажа и запуск первой очереди ускорителя (с одним клистроном на энергию 100 МэВ) сдерживаются недостатком финансирования. Завершена техническая подготовка к демонтажу реактора ИБР-30. Работа должна начаться весной 2005 года после получения разрешения на ввод в эксплуатацию построенного хранилища радиоактивных отходов. Доставлено топливо для размножающей мишени ИРЕН, что позволяет начать подготовку к ее изготовлению. Однако в целом из-за хронического недофинансирования проекта пуск первой очереди установки ИРЕН может ожидаться не раньше 2008 года.

На нейтронных спектрометрах ИБР-2 выполнено несколько интересных экспериментов. В частности, на рефлектометре с поляризованными нейтронами РЕМУР впервые исследовано явление сосуществования сверхпроводимости и магнетизма на границах раздела в тонких слоях сверхпроводящего соединения ($V/Fe_{0.66}V_{0.34}$) и ферромагнетика (Fe/V плюс двойной слой V/Fe). Изучено влияние сверхпроводимости на

магнитные свойства системы, которое сильно зависит от состава и структуры магнитного слоя. На малоугловом дифрактометре ЮМО определена структура поликарбоксильных дендримеров. Впервые выявлены особенности организации концевых групп дендримеров, в частности их слоистый характер. Данная особенность может объяснить наблюдаемые ограничения на рост дендримеров .

В течение года был выполнен ряд работ и получены интересные результаты в области ядерной физики: завершены измерения по программе коллаборации nTOF - изучение природы вибрационных резонансов в делении, индуцированном нейтронами, и получение сечений деления для решения проблем ADS-систем и сжигания ядерных отходов. На пучке ПФ1 реактора ИЛЛ (Гренобль) был проведен эксперимент по исследованию массово-энергетических корреляций в тройном нейтронно-индуцированном делении. В плане подготовки эксперимента по прямому измерению длины nn-рассеяния на импульсном реакторе ЯГУАР (Снежинск) были проведены измерения потока быстрых, эпитепловых и тепловых нейтронов по всей глубине (~ 12 м) подреакторной шахты. На реакторе ИЛЛ (Гренобль) был выполнен эксперимент по хранению УХН, в результате которого было показано существование канала аномальной утечки УХН в широком интервале температур (70-800 К) и из сосудов с совершенными стенками, выполненными из монокристаллического сапфира.

Продолжены исследования эффекта квантования энергии при дифракции ультрахолодных нейтронов на движущейся решетке. Как было показано ранее, решетка, движущаяся поперек направления распространения нейтронной волны, модулирует прошедшую волну по фазе и (или) амплитуде и выступает в роли нестационарного квантового устройства. Это явление было продемонстрировано в эксперименте, поставленном на реакторе ИЛЛ (Гренобль). Полученные результаты находятся в хорошем согласии с квантовомеханическим расчетом. Явление изменения энергии нейтрона при нестационарном воздействии на нейтронную волну открывает новые экспериментальные возможности, в частности, возможность фокусировки нейтронов во времени путем управляемого изменения их скорости. В недавних экспериментах работоспособность такой временной линзы была продемонстрирована. Эффективность фокусировки достигает примерно 30% и в дальнейшем может быть существенно увеличена.

Продолжено изучение атмосферных выпадений тяжелых металлов с применением техники биомониторирования, НАА и ГИС технологий (проект РЕГАТА) на территории России и ряда других стран. Проведен сравнительный анализ различных биомониторов (лишайников, коры деревьев) и почвы из района нефтеперерабатывающего завода в Румынии. Проведен НАА более чем 250 образцов растительного и животного

происхождения в рамках координационной программы (2002-2005) и проекта Технической кооперации с МАГАТЭ (2003-2005) по контролю и качеству продуктов питания, выращенных в условиях сильного антропогенного загрязнения. Продолжены совместные работы с группой биофизиков Института физики АН Грузии по разработке новых медицинских препаратов и сорбентов на основе сине-зеленой водоросли *Spirulina platensis.*

В заключение можно отметить, что наблюдается рост интереса стран-участниц ОИЯИ к работам в области нейтронных исследований. Важно, что в последние годы в Лабораторию пришло довольно много молодежи. Все эти факты дают уверенность, что несмотря на трудности Лаборатория продолжает успешно и динамично развиваться.

А.В. Белушкин

Директор

9марта 2005 года

1. SCIENTIFIC RESEARCH

1.1. CONDENSED MATTER PHYSICS

Main scientific results

Diffraction. With the help of combined analysis of X-ray and neutron (obtained with HRFD) diffraction data the crystal structure of the single-phase compound Li_2BeD_4 has been determined. The compound crystallizes in monoclinic syngony (space group $P2_1/c$) with lattice parameters a = 7.06228(9) Å, b = 8.3378(1) Å, c = 8.3465(1) Å, β =93.577(1)°, Z = 8. Its structure contains isolated tetrahedrons BeD_4 and Li atoms in between (**Fig.1**) and remains practically unchanged down to 8 K. Determination of the crystal structure of Li_2BeD_4 is the first real result for ternary Li-Be-H system. It has demonstrated the power of the state-of-the-art structural processing programs for direct determination of structures from powder diffraction spectra and the advantages of complimentary use of neutron and X-ray diffraction data to obtain structural information on the systems consisting of the lightest atoms.

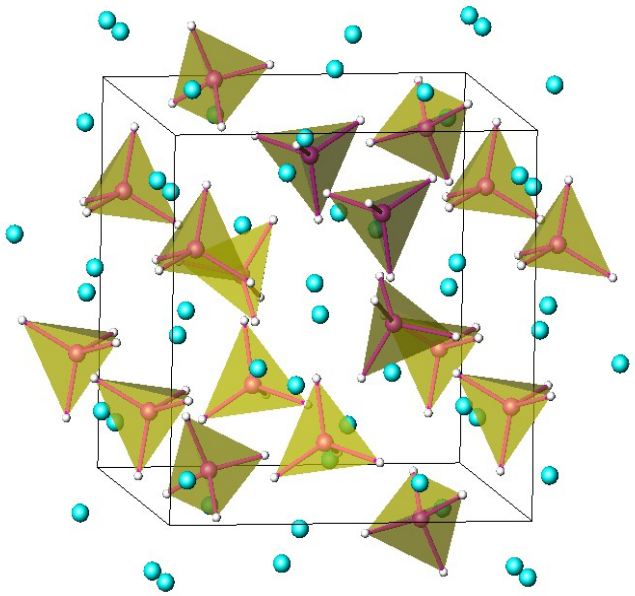

Fig.1. *Crystal structure of Li_2BeD_4 determined using neutron diffraction data.*

On the DN-12 diffractometer the effects of high pressures (up to 5 GPa) and low temperatures (in the range from 15 to 300 K) on atomic and magnetic structures of the manganites $Pr_{1-x}Sr_xMnO_3$ (x = 0.5, 0.56) have been studied. At normal pressure the compounds $Pr_{0.44}Sr_{0.56}MnO_3$ and $Pr_{0.5}Sr_{0.5}MnO_3$ have a tetragonal structure (space group I4/mcm). With decreasing temperature in $Pr_{0.44}Sr_{0.56}MnO_3$ a phase transition to the antiferromagnetic (AFM) phase of the A-type (**Fig.2**) accompanied by a structural phase transition from tetragonal to orthorhombic structure (space group Fmmm) is observed. In $Pr_{0.5}Sr_{0.5}MnO_3$ with decreasing temperature transitions to the intermediate tetragonal ferromagnetic (FM) and low-temperature orthorhombic AFM phase of the A-type are noted. At high pressures, $P \approx 2$ Gpa, in $Pr_{0.44}Sr_{0.56}MnO_3$ a new tetragonal AFM phase of the C-type appears and coexists with the original orthorhombic phase of the A-type in the region of low temperatures. In $Pr_{0.5}Sr_{0.5}MnO_3$ the effect of high pressures results in a significant increase in the temperature of the phase transition from tetragonal FM phase to orthorhombic AFM phase of the A-type. In the region of low temperatures the coexistence of the original orthorhombic AFM phase of the A-type with the tetragonal phase, which does not show evidence of the long-range magnetic order, is observed.

The scientific program at the EPSILON and SKAT diffractometers was focused on investigations of internal stresses in polycrystalline materials (mainly rocks), texture analysis of

rocks and determination of anisotropic physical properties of rocks from crystallographic textures. In particular, the studies of residual stresses in marble-based construction materials aimed at gaining a better understanding of the processes causing deformations in various constructions have been carried out.

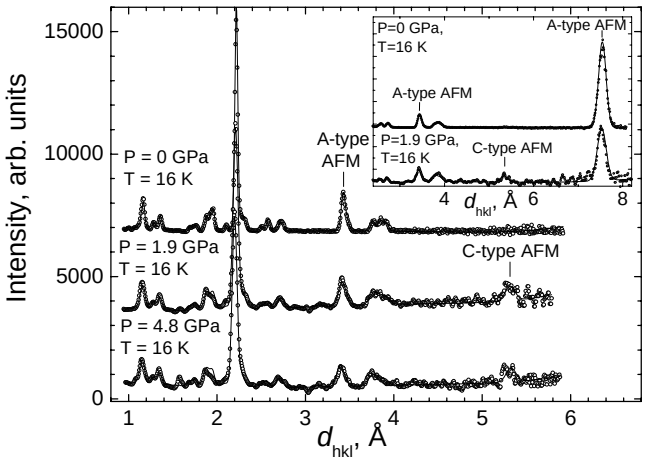

***Fig.2**. Sections of neutron diffraction spectra of $Pr_{0.44}Sr_{0.56}MnO_3$ obtained at high pressures P = 0, 1.9 and 4.8 GPa, T = 16 K and treated by the Rietveld method. With increasing pressure a new AFM phase of the C-type was observed.*

For the first time the dynamics of the α-β-transition in a rock sample (quartzite) has been studied by means of neutron diffraction and acoustic emission (AE). The values of internal stresses were estimated basing on the detected changes in interplanar spacings of the crystalline lattice during the α-β-transition (**Fig.3**). They were found to be several times higher than the mechanical stresses applied to the sample (**Table 1**). Upon completion of the α-β-transition there appeared flashes of AE with the intensity two orders of magnitude higher than the mean level of AE caused by thermal cracking of the sample on heating. The occurrence of outbreaks of elastic AE vibrations during a phase transition in quartz, a rockforming mineral of the Earth crust, points to a discrete behavior of the observed instability. It is not improbable that such phenomena may contribute to the development of an earthquake center as a consequence of changes in the strained state of the medium or a trigger effect.

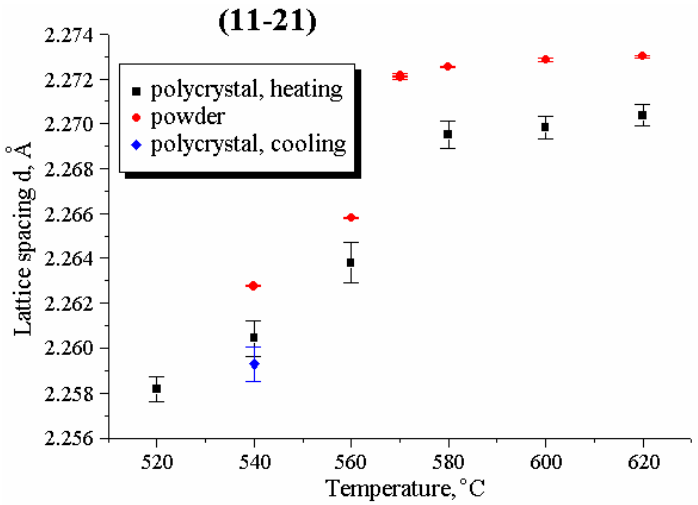

***Fig.3.** Temperature dependence of interplanar spacing (11-21) in quartz powder and polycrystal (heating and cooling*

Table 1

Internal micro- ($\sigma_{LATTICE}$) and macro- (σ_{MACRO}) stresses in quartzite in the region of α – β transition.

(*hkil*)	T, °C	Δd/d, $*10^{-3}$	Young modulus E, GPa	$\sigma_{LATTICE}$, MPa	σ_{MACRO}, MPa
$(10\bar{1}0)$	540	1.24	76.3 84.0	94.6 104.2	-25
	600	0.03	116.4 110.7	3.5 3.3	-27
$(11\bar{2}1)$	540	1.00	76.3 84.0	76.3 84.0	-25
	600	0.14	116.4 110.7	16.3 15.5	-27

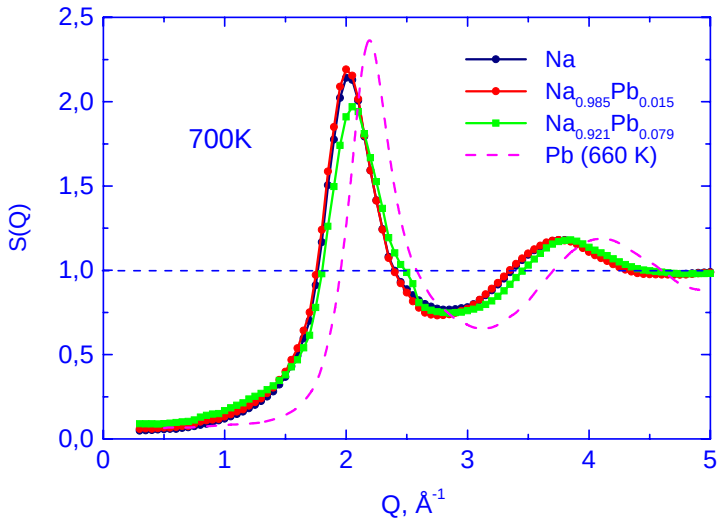

***Fig.4**. Structural factors of liquid sodium and Na–Pb melts.*

Inelastic scattering. On the DIN-2PI inelastic scattering spectrometer a comparison of the experimental data for the system sodium-lead with the calculated spectra has been performed (**Fig.4**) basing on the molecular dynamic simulations. It has been concluded that at low concentrations of the admixture, C_{Pb} ~10 a.w. % and lower, there are no Na_4Pb-type clusters in significant quantities, and dissolved lead is present in the atomic state in the melt. This conclusion makes it possible to estimate the thermodynamical and physical-chemical parameters of the melt more correctly.

On the NERA-PR spectrometer the experiments and modeling of the vibration state density function in solid methanol with different types of deuteration (CH_3OH, CH_3OD, CD_3OH, CD_3OD) have been carried out (**Fig.5**). It has been demonstrated that solid methanol may be effectively used as a standard to estimate the quality of computer simulations of molecular dynamics both in crystalline and amorphous phases.

Polarized neutron reflectometry. On the REMUR polarized neutron reflectometer the phenomenon of superconductivity and magnetism on the interface of a superconductor and a ferromagnet has been studied. In particular, layer structures with coexisting periodic structures Fe/V plus bilayers V/Fe and V/$Fe_{0.66}V_{0.34}$ composed of superconducting layers of vanadium and ferromagnetic layers of iron have been investigated (**Fig.6**). The effect of superconductivity on

magnetism has been demonstrated to depend strongly on the composition and structure of the magnetic layer.

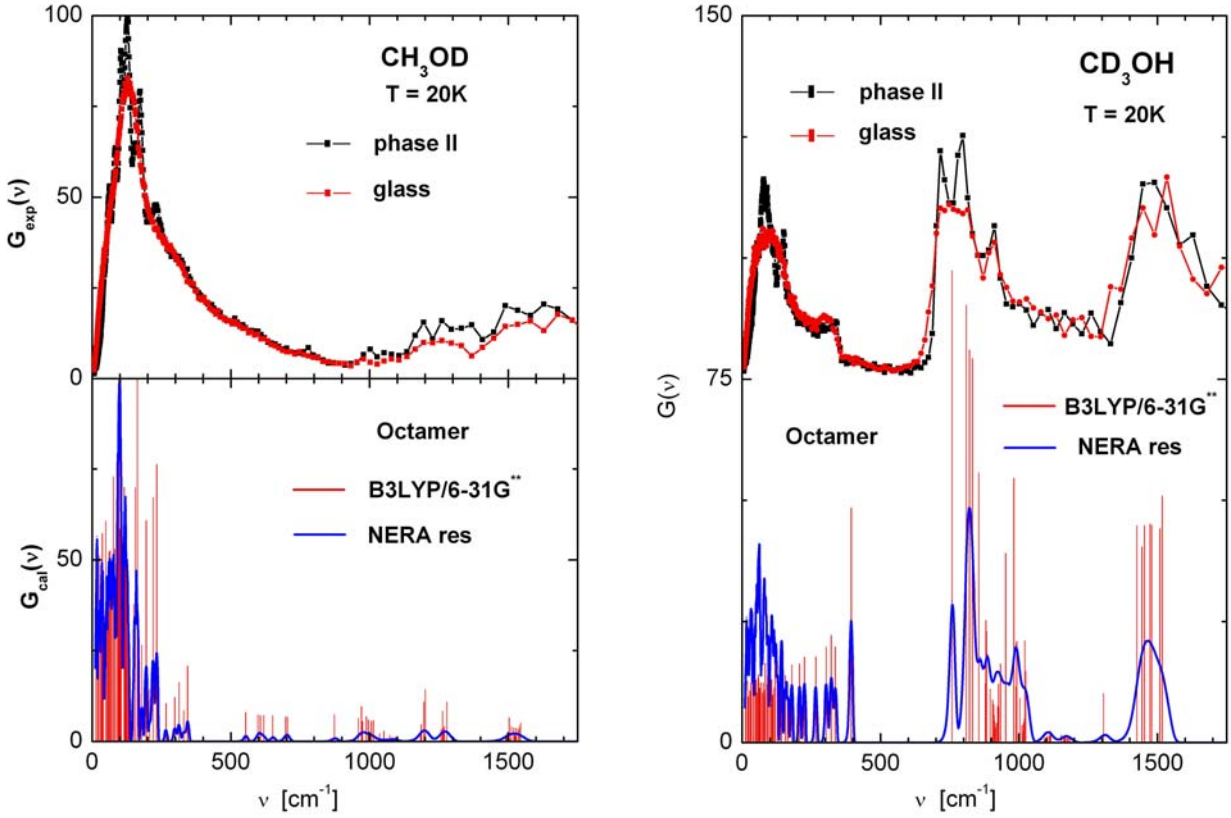

Fig.5. *Isotopic and structural effects on vibrational spectra of methanol.*

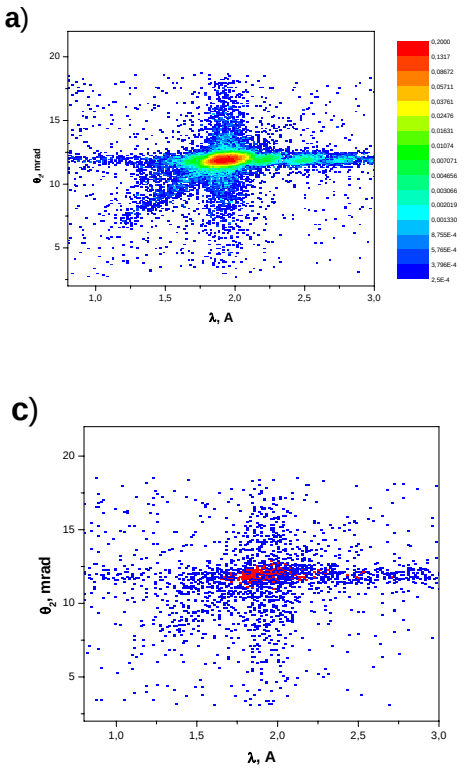

Fig.6. *The $R^{+}{}^{+}$ coefficient of diffuse reflection from the structure Pd(2 nm)/V(36.5 nm)/17[Fe(1ML)/V(1ML)]/10[Fe(4.7 nm)/V(4.7 nm)/MgO depending on the scattering angle θ_2 and the wavelength λ in the vicinity of the first Bragg maximum. The external magnetic field is 0.7 kOe. (a) Experimental reflection coefficients for measurements at T=1.6K; (b) model calculation for T=1.6K; (c) difference between the experimental reflection coefficients for T=1.6K and T=7K. Red color corresponds to positive values and blue color to negative values.*

Small-angle neutron scattering. On the YuMO small-angle neutron scattering setup a number of polymeric systems, dendrimers, as well as mixed solutions of polymers and surfactants have been studied. The studies of the structure of polycarbosilane dendrimers with different molecular structures have revealed structural peculiarities of stacking of end groups of dendrimers, namely their layered character. This may account for a restraint in the growth of dendrimers with increasing generation degree.

Small-angle neutron scattering experiments with contrast variation on highly stable water-based magnetic liquids have been conducted. The parameters of colloidal particles of liquids at various concentrations of dispersed magnetic substance (magnetite) have been obtained (**Fig.7**). The structure of the given liquids has been compared with less stable water samples that use other surfactants for stabilization, as well as with highly stable magnetic liquids on the basis of nonpolar carriers, such as benzol.

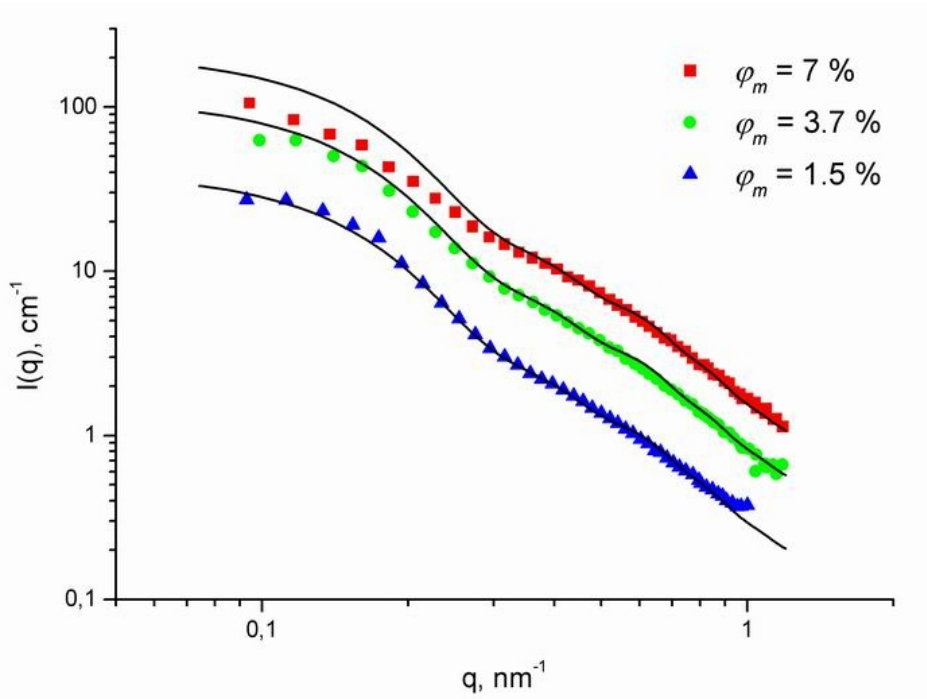

***Fig.7**. Experimental data of small-angle scattering by the magnetic liquid Fe_3O_4/DBS+DBS/D_2O at various volume fractions of magnetic materials, φ_m. The magnetite was produced by chemical condensation. The stability of the system is realized by a double layer of dodecylbenzenesulfonic acid. The lines correspond to the calculation curves according to the "core-shell" model for non-interacting particles. The interaction effect does not manifest itself up to φ_m=4 %. The deviation of the upper experimental curve from the model one at small q values reflects "soft" interaction between colloidal particles.*

The coagulation of water dispersions of fullerenes on addition of various salts has been investigated. Also, the time evolution of the absorption spectra of visible and ultraviolet radiation has been analyzed. The concentration of fullerenes in solutions has been found to decrease monotonically on addition of salt. This confirms a charge character of stabilization of colloidal particles in the given systems. The measured coagulation thresholds differ significantly from the data reported earlier. The experiments and preliminary treatment of the data on small-angle neutron scattering from coagulating water solutions of fullerenes in a real time mode have been carried out. The dynamics of growth of fullerene clusters and their concentration in solutions on coagulation have been estimated.

Neutron diffraction studies of the structure of *Stratum Corneum* model membranes have been carried out. The structure of the mixed four-component system ceramide 6/cholesterol/

palmitic acid/cholesterol sulfate with various weight ratios of components and a low level of hydration has been investigated. The position of cholesterol in a lipid bilayer has been determined. The distribution function of water in the bilayer has been measured. It has been established that *Stratum Corneum* model membranes have low hydration of the intermembranous space as compared to phospholipids.

Main methodological results. The modernization of the REMUR reflectometer at the IBR-2 pulsed reactor has been carried out. As a result, the radiation background in the spectrometer has been reduced and the intensity of the neutron beam upon leaving a multichannel polarizer has increased. In the spectrometer the design of two mirror-polarizers is realized, which makes it possible to considerably increase the neutron beam polarization. The new software for the spectrometer based on the use of a VME-PSI adapter has been designed to enhance the performance reliability.

The modernization of the REFLEX reflectometer has been performed. Test measurements on the setup in September-October, 2004 demonstrated that as a result of a shift of the mechanical chopper the working part of the thermal neutron spectra increased from $\Delta\lambda$=5Å to 10Å, which considerably extended the range of the detected values of momentum transfer of the scattered neutrons.

In accordance with the plan, on the DIN-2PI spectrometer the designing of a new case of the TS-3000M thermostat has been completed. The design drawings for the modernized variant of a shell for the thermostat case have been worked out. The unit of the radiation screens has been reconstructed. The application of new materials, specifically tungsten-rhenium alloys, that are more practically executable than alloys based on pure tungsten, has made the construction more convenient for varying the number of screens and their materials and thickness depending on the parameters of experiments.

On the REMUR reflectometer a new algorithm for the implementation of the different theoretical approaches to calculate diffusion scattering in neutron reflectometry experiments has been developed. The computer software packages for model calculations and fitting of experimental data on neutron scattering from magnetic multilayered nanostructures have been designed. New programs allow one to process the experimental data more correctly and to study proximity effects in the scale interval of $1 \div 10^4$ nm.

In the biophysical research group the software to describe the inner membrane structure of lipid vesicles using small-angle neutron scattering data has been designed. The computer programs are based on the hydrophobic-hydrophilic model of bilayers with a linear function of water distribution and on the model of separated form-factors. The work of the software has been demonstrated on several lipid systems studied experimentally by means of small-angle neutron scattering.

1.2. NEUTRON NUCLEAR PHYSICS

Introduction

In the course of the year 2004 the main work in the field of neutron nuclear physics was carried out at EG-5 in FLNP JINR and on neutron beams in other nuclear centers of Russia, Bulgaria, Poland, Czech Republic, Germany, Republic of Korea, China, France, USA, and Japan. The studies were in traditional directions, such as the investigation of time and spatial parity violation processes in the interaction of neutrons with nuclei, studying of the quantum-mechanical characteristics and dynamics of the fission process, experimental and theoretical investigations of the electromagnetic properties and beta-decay of the neutron, gamma-spectroscopy of neutron-nuclear interactions, studies of atomic nucleus structure, obtaining of the new data for reactor applications and nuclear astrophysics, experiments with ultracold neutrons, and applied investigations.

1. Experimental investigations

1.1. Spatial and time parity violation in the interaction of neutrons with nuclei

1.1.1 Search for and investigation of the structure of subthreshold neutron p-resonances in lead isotopes by the combined correlation gamma spectroscopy method

During the reported year the analysis of the data obtained in the experiments conducted in 2002–2003 to search for the negative neutron p-resonance in lead isotopes with the aim of explaining of the earlier discovered spatial parity violation effect that demonstrated itself as rotation of spin of polarized thermal neutrons on their transmission through the sample has been completed. With the purpose of refining the obtained results that provide evidence of the existence of a strong p-wave resonance in the isotope ^{207}Pb but not in ^{204}Pb as expected from the results of the previous works by the ITEP group, the preparation of the gamma-spectrometer COCOS for reconstruction to increase its efficiency and processing speed has been conducted.

1.1.2 Preparation for investigations of T-noninvariance effects in neutron nuclear interactions

The development of the measuring procedures of T-noninvariance effects in neutron nuclear interactions continued. The measurement of three-vector P-odd T-odd and five-vector P-even T-even correlations of the **I, k, s** vectors is considered to be the most promising. For the study of the five-vector correlation an aligned nonpolarized target with nuclei having p-resonances in the energy region up to 100 eV is required. And the investigation of three-vector correlation requires a polarized nuclear target with p-resonances where P-odd effect was observed. The experiments of this kind should be performed at intense neutron sources. In this connection the work in this area has been carried out in two directions:

I. For the purpose of studying the five-vector correlation the aligned nuclear target can be obtained by the static method that uses the quadrupole interaction of nuclei with a crystal field at low temperatures, or, probably, with the use of the recently suggested method of dynamic nuclear alignment. For the static method the alignment of ^{127}I nuclei in a monocrystal of iodine at low temperatures was estimated. It was found that the alignment suitable for measurements (~50%) can be achieved by cooling the iodine monocrystal to ~20-50 mK. To verify the idea of the dynamic alignment of nuclei, the following has been done:

- In cooperation with ITEP a monocrystal of lutetia niobite with a paramagnetic admixture was prepared.
- The EPR-spectra of the crystal were measured.

- A trial run of dynamic alignment was performed, which showed the necessity of the creation of a more sensitive, wide-range Q-meter that would not destroy the alignment.
- At present, the creation of this Q-meter is under way.

II. For the investigation of the three-vector correlation a polarized lanthanum target is considered to be the most promising, since in a p-wave resonance of ^{139}La at an energy of 0.75 eV a considerable P-odd effect has been observed. An appropriate polarized target using a $LaAlO_3$:Nd+ monocrystal is to be created in cooperation with KEK (Japan). At present, the group has a monocrystal sample $LaAlO_3$ granted by the Japanese party for carrying out the experiments to obtain the polarized target. Neutron diffraction studies of the crystal structure of this sample have been conducted and showed its applicability for performing trial experiments of the dynamic polarization of ^{139}La nuclei.

1.1.3 Current status of the KaTRIn project

Within the framework of cooperation with KEK (Japan) the setup for the measurement of ^{3}He polarization by the neutron transmission method has been modernized. The modification has been made for the purpose of the measurement of the pseudomagnetism of the polarized nuclei ^{129}Xe and ^{131}Xe. A schematic view of the modified setup is given in **Fig.1**.

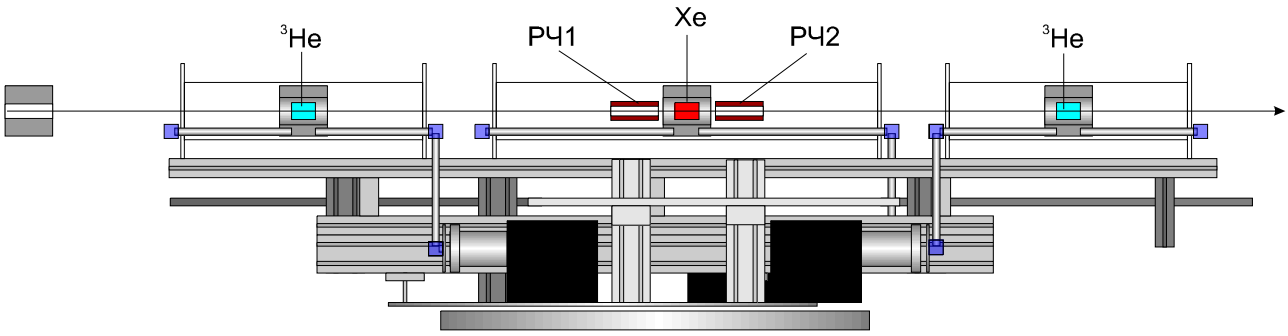

Fig. 1. *A schematic view of the experimental setup.*

In the Figure the neutron beam is directed from left to right. The left cell with polarized ^{3}He serves as a neutron polarizer. Upon leaving the cell, neutrons are polarized along the beam direction. A radio-frequency coil RF1 rotates the polarization of neutrons about the vertical axis so that at the point of entry into the cell with polarized Xe (natural mixture of isotopes) it is perpendicular to the plane of the Figure. A radio-frequency coil RF2 rotates the neutron polarization back towards the beam direction and the right cell with polarized ^{3}He serves as a polarization analyzer.

The pseudomagnetic interaction of polarized neutrons with polarized Xe nuclei must result in the rotation of the plane of polarization of the beam. In this case the experimental effect should demonstrate itself as a difference in the counts of the detector for the measurements with polarized and unpolarized Xe. In practice, the difference in the transmission of the polarized neutron beam in the region from 0.02 to 0.1 eV is to be measured.

^{3}He and odd Xe isotopes are polarized by the optical pumping method (optical parts of the setup are not shown in the Figure).

At present, the setup is being tested on a neutron beam.

1.1.4 Creation of a polarized proton target

Continuous and discrete silver heat exchangers of a ^{3}He in ^{4}He dilution cryostat with a superconducting solenoid have been manufactured and tested. The cryostat is intended for nuclear polarization by the "brute force" method and dynamic pumping of polarization. The ^{3}He in ^{4}He

dilution system has been assembled. The cryostat has been tested and its parameters have been determined. The outcomes of the trial:

- minimal temperature on a sample T = 24 μK
- circulation rate n= 0.98 μmol/s
- magnetic field intensity in the center of solenoid H= 5.8 T at the homogeneity of a magnetic field $\Delta H/H= 10^{-4}$

For the polarized proton target the titanium hydride TiH_2 plates 14 mm in diameter and 0.2 mm thick have been manufactured by pressing the titanium hydride powder under a pressure of $2\cdot10^6$ g/cm^2. On beam №1 of the IBR-2 reactor at the polarized neutron spectrometer the works to install the polarized nuclear target are being completed.

1.2 Neutron-induced and spontaneous fission

1.2.1 Experimental investigation of ternary fission of ^{235}U on the cold neutron beam of the reactor in ILL (Grenoble)

In 2004 on the beam PF1 of the reactor in ILL (Grenoble) an experiment to investigate the neutron-induced ternary fission of ^{235}U was conducted. The experiment was performed in collaboration with the scientists from the Flerov Laboratory of Nuclear Reactions, PNPI (Gatchina), Germany and France. This experiment was a continuation of a series of works carried out on spontaneous ^{252}Cf sources to investigate the ternary fission process. The purpose of this experiment was to study mass-energy correlations of fission fragments and light charged particles for the lighter fissionable system, which is ^{236}U*.

The fission fragments were measured by a fast double ionization chamber with a sectorized cathode allowing the determination of energy, mass and the escape direction of fission fragments, and the light charged particles were detected with high resolution ΔE-E telescopes, which make it possible to identify the particles by their charge and mass ranging from the isotopes of hydrogen to beryllium as well as to measure their energy and angular distributions. In the course of 20 days of beam time about 4×10^7 events with emission of α-particles, 3×10^5 events with emission of ^{6}He, 1×10^4 events with emission of Li isotopes and 6×10^3 events with Be isotopes were accumulated. There were obtained preliminary results on the yield, energy and angular distributions of light charged particles, as well as the mass and energy distribution of fission fragments for various modes of ternary fission. This experiment also makes it possible to investigate some properties of quaternary fission with simultaneous emission of two α-particles or an α-particle and tritium. The example of energy distributions of fission fragments for two modes of quaternary fission is given in **Fig.2.**

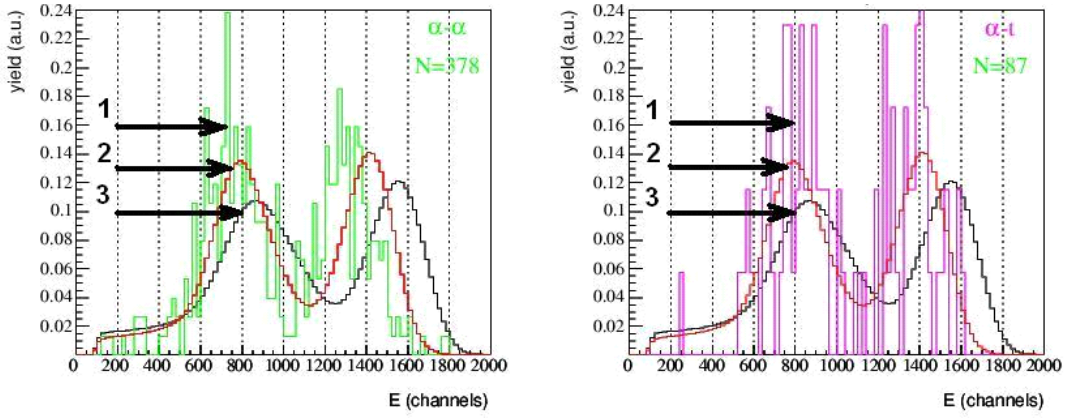

***Fig. 2**. Energy distributions of fission fragments (raw data) for quaternary fission of $^{235}U(n_{th},f)$ with emission of two α-particles (left) and an α-particle and tritium (right) – histogram 1. Histogram 2 corresponds to the ternary fission with emission of an α-particle, histogram 3 to binary fission.*

1.2.2 Investigation of neutron-neutron correlations in spontaneous fission of ^{252}Cf

In the framework of preparation to the experiment to study neutron emission in ternary fission of ^{252}Cf as well as to search for scission neutrons and to study neutron-neutron correlations, a test experiment using the multisectional neutron detector DEMON was carried out in Strasbourg (France). In the experiment a spectrometric ^{252}Cf source on a thin nickel substrate was used. It was placed in a double ionization chamber that makes it possible to determine energy, mass and escape direction of fission fragments. Fission neutrons were detected by the DEMON neutron detectors arranged at different angles to the axis of the fission chamber (see **Fig.3**).

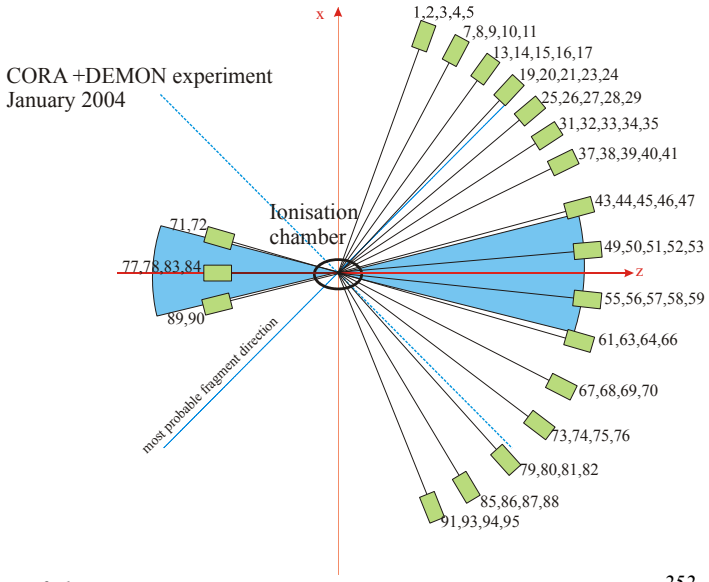

***Fig. 3**. The layout of the experiment to investigate neutron escape in ^{252}Cf fission.*

The detectors made it possible to differentiate neutrons from gamma-quanta by the pulse shape, as well as to determine neutron energy by the time of flight and exit angle. In the process of preliminary data treatment the known results on angular and energy distributions of neutrons for ^{252}Cf were reproduced and thus the experimental technique was tested and improved. About 10^6 neutron-neutron correlations were accumulated. The investigation of these correlations together with mass-energy and angular distributions of fission fragments might help to find the correlation unobserved earlier of neutron emission and spin direction of fission fragments, which in its turn can throw light on the nature of formation of spins of fission fragments. It seems unlikely that we shall manage to obtain this information from the test experiment, because the fission source substrate was damaged in transit. Similar investigations are planned to be carried out in the future experiment scheduled for the end of 2005.

1.2.3 Measurement of delayed fission neutron yield

To continue works aimed at obtaining data on the yields and decay constants of groups of delayed neutrons in the fission of minor actinides, the positioning of a mirror neutronguide on beam 11B of the IBR-2 reactor has been carried out. The experimental technique to study characteristics of delayed fission neutrons of the ^{246}Cm compound nucleus has been developed, which makes it possible to conduct investigations at the expected level of spontaneous fission neutron background. An ionization fission chamber with ^{245}Cm isotopes has been assembled. The integration tests of the modernized «Izomer» setup that comprises data acquisition and accumulation systems and control units of the neutron beam chopper, have been performed. The first measurements of ^{235}U and ^{239}Pu have been conducted with the modernized setup.

1.3 Gamma-spectroscopy of neutron-nuclear interactions

1.3.1 Investigation of two-quantum gamma-cascades

The problem of completely model-absent determination of the density of levels in a fixed interval of their spins and reduced probability of their exciting and discharging dipole electric and magnetic gamma-transitions at excitation energies around the neutron binding energy has been solved. No analogous experimental data exist in the world.

The employed method uses the experimental data on the cascade population of levels excited at thermal neutron capture up to the excitation energies of no less than 3-5 MeV and the intensities of the earlier measured two-quantum cascades to the low levels of the same nuclei. A comparison of these data makes it possible to estimate experimentally the degree of the difference in the energy dependence of the radiative strength functions of the primary and secondary transitions in the cascade gamma-decay of the compound state and, with accounting for the difference, to determine, without any additional hypotheses, the interval of probable densities of levels with a minimum systematic error to date. Such data were obtained for 19 nuclei from the region $39<A<201$. The main physical conclusion that follows from their analysis is: in the majority of nuclei a quite essential change in the structure of the excited levels is observed in the regions around 20, 50 and 80% of the neutron binding energies. The effect manifests itself in a considerable change of the derivative of the energy dependence of level densities and the variation (well-correlated with its change) of the radiative strength functions of both primary and secondary gamma-transitions.

Within the framework of the existing models of level density the observed effect may be related to the breakup of at least two Cooper pairs of nucleons. But the magnitude of the effect of the change of the observed density of levels depending on the excitation energy of a nucleus does not correspond to the predictions of the generalized model of the superfluid nucleus first of all by the position of a point of superfluid-to-ground-state phase transition.

1.3.2 Determination of the level scheme of Yb isotopes

In 2004 in the framework of the cooperation between FLNP and the scientists from the Prague Polytechnic University (Prague) the analysis of the results obtained in the experiments on the filtered neutron beams conducted at the pair spectrometer in the Brookhaven National Laboratory continued. Gamma-spectra of radiative capture of thermal neutrons, neutrons with energies of 2 keV and 24 keV have been obtained. These spectra have been treated and a considerable amount of information on the levels of a ^{174}Yb nucleus has been gained. About 300 levels have been revealed up to an excitation energy of 4 MeV. The paper «Levels of Populated ^{174}Yb in Individual Resonance Neutron Capture» has been prepared to publication on the basis of the results of the measurements carried out in FLNP JINR at the IBR-30 reactor, in which gamma-spectra from 32 resonances of ^{173}Yb were obtained. The paper lists the values of energy, spin and parity of 77 levels of a ^{174}Yb nucleus and compares the obtained results with the available data.

1.4 Investigations of (n, p) and (n,α) reactions

At the EG-5 generator of FLNP JINR experiments to measure the energy dependence of the angular distribution coefficients in the reaction ^{14}N(n,p)^{14}C for the neutron energy interval ~ 10 keV ~ 1 MeV started. Investigations of the interference effects of s- and p-resonances in the reaction (n,p) are of interest both from the viewpoint of obtaining more complete spectroscopic information about p-resonances and more precise interpretation of the measurement results of P-odd effects. Neutrons were produced in the reaction ^{7}Li(p,n)^{7}Be. A thick lithium target and protons with an energy exceeding the threshold value by 20 keV were used. Thus, the integrated neutron spectrum was formed in the cone of ~ 120°, which was in the energy dependence close to the Maxwellian distribution at an average energy of ~ 30 keV. The angular distribution data for such spectra are also

of importance for the understanding of what causes so strong discrepancies (by a factor of 2-3) in the Maxwellian spectrum-averaged cross section values at stellar temperatures obtained in a number of works. The detection and spectrometry of protons were performed by a two-section ionization chamber with a grid and electronic multidimensional data acquisition system. An adenine ($C_5H_5N_5$) 267 μkg/cm^2 thick target of sizes 180×160 mm was used as a sample. The forward-backward correlation $\alpha_{fb} = (4.2 \pm 4.0)\cdot 10^{-2}$ not accounting for the background was obtained.

At present, the design of the device for rotating and moving the chamber to perform the main measurements and estimations of the background is being developed.

The ^{6}Li and Be targets for joint experiments to study the (n,α) reaction at the Peking University have been manufactured. A gas deuterium target is being designed to continue the investigations of the (n,p), (n,α) reactions on fast neutrons at EG-5.

The work on preparation to the investigation of "nonstatistical" effects in α-decay of neutron resonances of ^{147}Sm at the slowing-down time spectrometer STS-100 in INR RAS in Troitsk has been started.

1.5 Nuclear data program

1.5.1 Investigation of resonance structure of neutron cross-sections

The treatment of the time-of-flight spectra earlier obtained on 122 m, 501 m and 1006 m flight paths of the IBR-30 reactor with the help of multisectional neutron and gamma-ray detectors for Nb, Mo, Pb, ^{235}U (77 K and 293 K) sample filters has continued through the past year. From the time-of-flight spectra after the background subtraction the total and partial neutron group cross-sections and the resonant blocking coefficients of the total cross-section and the scattering cross-section in the energy range from 100 eV to 200 keV for Nb, Mo, Pb have been determined. The experimental errors of cross-sections and blocking coefficients are 3-7% and 8-15%, respectively. The analogous values have been obtained using the GRUKON program on the basis of the estimated data of various libraries. By and large the calculated and experimental data coincide, but in some energy groups the discrepancies fall outside the limits of experimental error.

For uranium-235 from the time-of-flight spectra of different multiplicities of gamma-ray coincidence after the subtraction of background components the Doppler effect has been determined for the alpha value at temperatures of 293 K and 77 K. The experimental errors for the alpha value are 2-10% depending on the resonance peculiarities of the alpha value. The alpha value has been calculated on the basis of the estimated data of various libraries using the GRUKON program. The discrepancies of the calculated and experimental values amounts to as much as 30% in some resonances and energy groups. The final results of these investigations have been presented at the international scientific seminars and conferences in Russia, Romania, Poland and Turkey. These works have been conducted in the framework of cooperation between FLNP (Dubna), IPPE (Obninsk), INRNE BAS (Bulgaria) and University of Lodz (Poland).

Work has continued to create a facility at the IBR-2 reactor for monochromating thermal and cold neutrons and for shortening fast neutron pulses with the help of mechanical neutron choppers. The measurements of total cross-sections have been carried out on beam 6B at IBR-2 in the cold neutron region.

1.5.2 Nuclear data for ADS and studies of fine structure of threshold vibrational resonances

Within the last three years at the n_TOF neutron source of CERN within the framework of wide international collaboration together with the colleagues from IPPE (Obninsk) the (n,f)-cross-sections with highly enriched isotopic targets of a number of actinides have been studied in a wide neutron energy range. The research program has been aimed at obtaining new data (or refining of the available data) for accelerator driven subcritical systems (ADSS), as well as at studying fundamental aspects of nuclear fission.

In 2004 the measurements were carried out with the fast ionization chamber FIC1 for ^{241}Am, ^{243}Am and ^{245}Cm samples using ^{235,238}U targets as reference ones. In addition, with the help of the modernized ionization chamber FIC0 complemented by a grid that makes it possible to measure (along with the (n,f)-cross-section) a difference in the yields of fission fragments along and opposite the neutron beam direction (the so-called forward-backward angular correlation) the measurements with a ^{236}U sample have been performed in a neutron energy range up to 1MeV. The data obtained in October and November of 2004 have been analyzed together with the data from the measurements carried out in 2002-2003 for ^{234,236}U, ^{232}Th, ^{237}Np samples. Some preliminary results for a neutron energy range up to 1 Mev are presented below.

The ^{234}U (n,f)–cross-section measured at the n_TOF source (CERN) appears to be in satisfactory agreement with ENDFB data down to 1.5 keV. Owing to excellent energy resolution of the source a lot of new second well levels have been observed for higher energies. In addition, the reliable evidence for the existence of fine structure of threshold vibrational resonances has been obtained (see **Fig.4a**).

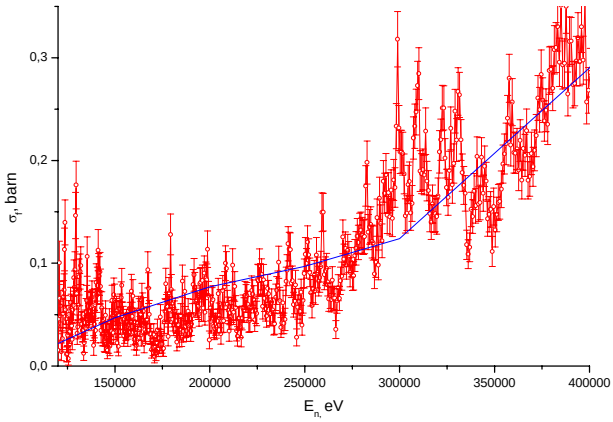

Fig. 4a

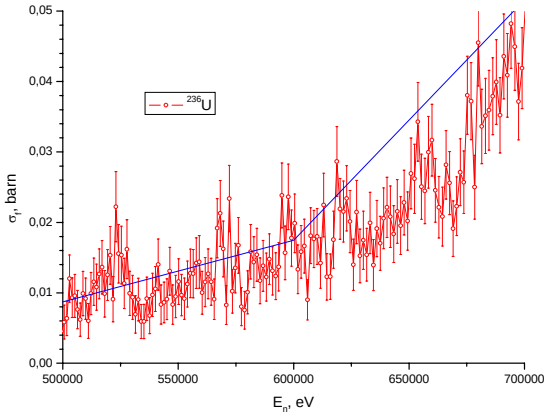

Fig. 4b

Very interesting results have been obtained for a ^{236}U target. Significant discrepancies between our results and the ENDFB data have been revealed. In particular, no resonances have been observed between 5 eV and 1.2 keV, whereas the ENDFB file gives several tens of them. In addition, for the resolved triplet in the vicinity of 1.2 keV a striking effect of resonance enhancement of fission barrier penetrability has been found. As for the ^{234}U (n,f)-reaction, in the case of a ^{236}U nucleus the existence of a fine structure of vibrational resonances in the vicinity of the fission threshold (as illustrated in **Fig.4b**) has been reliably confirmed.

For a ^{237}Np target our data are also in poor agreement with the ENDFB data. The difference in the fission cross-sections amounts to a factor of six in the neutron energy range in the neighborhood of 40 eV. This results in a change of the resonance integral for ^{237}Np(n,f)-reaction, which is an important value for a lot of waste transmutation systems. In addition, in the energy range from 500 to 700 keV the difference between the ENDFB data and the n_TOF cross-sections is about 7%, which is also of importance in estimating the neptunium balance in fast reactors. For the first time a lot of new levels of the second well for a ^{238}Np compound-nucleus have been observed above 500eV. These data will allow us to specify characteristics of fission barriers for a given nucleus and to gain a better insight into the relation between compound-levels of the first and second deformation wells.

1.6 Fundamental properties of the neutron

1.6.1 Investigation of neutron diffraction in gases

An important way of studying interatomic interactions is the observation of neutron diffraction in gases and liquids and determination of their structural factors $S(q)$ ($\hbar q$ - momentum transfer). When deriving $S(q)$ from experimental scattering data various corrections are introduced, including the n,e-interaction contribution to the scattering, which is assumed to be known. A new method for determining the n,e-scattering length b_{ne} developed last year and published in the JINR Communications E3-2003-183 and P3-2003-232 is based on the fact that the diffraction intensity $S(q)$ to a first approximation is proportional to the gas atom density n (its pressure), and the relative contribution of n,e-scattering does not depend on the gas density. And in inverse order, using the literature data on $S(q)$ of krypton at various n and the information on corrections, the initial scattering intensities have been obtained, the treatment of which has made it possible to reliably determine the n,e-scattering effect. However, because of the uncertainty of normalization constant in the description of absolute scattering intensities, a trustworthy value of b_{ne} has not been obtained.

In 2004 a way to avoid the difficulty connected with incomplete information on the corrections was found. A mathematical description of $S(q)$ data with b_{ne} as a free parameter was obtained. All data up to the largest n values were used and the model contained a term with n^2. The diffraction was described by choosing functions, which provided the required oscillations of $S(q)$ damping with increasing q and containing four free parameters in each term with n and n^2. The tenth free parameter was the above-mentioned normalization constant.

Simultaneous variation of ten parameters during the fitting to 1326 values of $S(q)$ (78 different q-values at 17 different n) resulted in $b_{ne} = -(1.53\pm0.24)\cdot10^{-3}$ Fm. This result is new, while its accuracy is modest. Its reliability (i.e. absence of large systematic errors) is determined by the reliable $S(q)$ data used.

1.6.2 Measurement of the n,e-scattering length

The construction of a new setup for measuring b_{ne} by a classical method that had been suggested by Fermi, but with the application of the time-of-flight method that enhances the reliability of results many times, has progressed to its practical stage. The setup comprises four neutron detectors, which have been manufactured and adjusted. Each of them is a proportional ^{3}He-counter with a pressure of ~ 8 atm equipped with a preamplifier and shielded by borated polyethylene and cadmium. Test measurements have been made with one of the detectors in Troitsk on a vertical neutron beam from a test target.

Working drawings of a positioner-rotator have been designed, with the use of which an axis of the scattering chamber will be brought into coincidence with an axis of a beam (vertical and horizontal), and then during measurements the scattering chamber with the detectors will be periodically rotated through 180°, so that each detector will alternately detect forward and back scattering.

Successful experience in describing the diffraction part of scattering by mathematical formulas and a wish to deal with as great electron form-factor difference as possible have done much to support the development of the project of a new experiment. For its realization a low density of gas (with a pressure of 1-3 atm) would suffice, but the energy of a monochromatic neutron beam should be within ~50-200 meV (λ ~ 1.3 - 0.6 angström). Then for back scattering angles the momentum transfer may amount to as much as ~ 10-20 inverse angström and correspondingly the form-factor values (0.36-0.19 for krypton) can be rather small.

Simultaneously, to eliminate the effect of detector efficiency spread, instead of vanadium as a standard scatterer an inert gas (neon) with smaller contribution of n,e-scattering is proposed to be used, which gives effect from thermal motion of atoms of the same nature as a base working gas.

1.6.3 Experiment of the direct measurement of the neutron-neutron scattering length at the pulsed reactor JAGUAR (Snezhinsk)

To verify the calculations and to choose an optimum variant of under-reactor shielding, test measurements have been conducted. For test measurements the following units and systems have been manufactured:

- regular moderator, regular head moderator and components of the under-reactor shielding made of borated polyethylene and tubular collimators;
- detecting system consisting of thermal and fast neutron detectors – gas proportional counters with ^{3}He and ^{4}He with preamplifiers;
- neutron detector position remote control system inside the channel.

A scheme of test measurements is given in **Fig.5**. A moderator, thick conical collimator and under-reactor shielding here are the same as in a real experiment, but without a vacuum channel and collimation system. Detectors in the under-reactor shaft can be positioned in any place of the shaft.

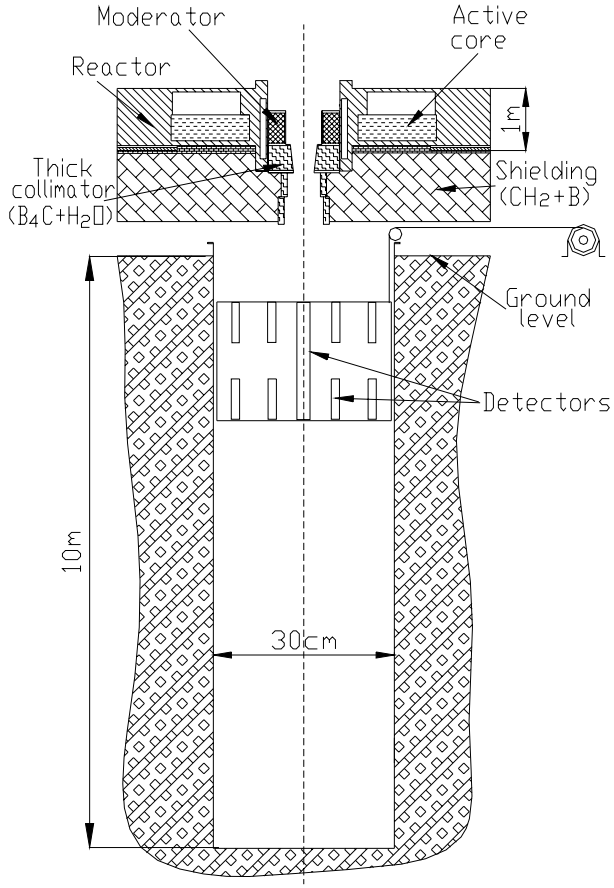

***Fig.5**. Scheme of test measurements.*

The measurements were carried out in the steady-state operating mode of the reactor. The flux densities for three groups of neutrons were measured: for thermal neutrons – with an energy below cadmium resonance, for epithermal neutrons – with an energy above cadmium resonance and for fast neutrons – with an energy of ~ 1 MeV. The measurements were carried out along the whole length of the shaft, for three various geometries and collimator types in order to gain more information for comparison of calculation data with experimental results. **Figure 6** presents preliminary results for the thermal neutron flux density dependence on the shaft depth for two different geometries of the collimator. As may be seen from the figure, the calculation data are in good agreement with the measurement data.

Measurements of low-energy neutron flux density are of interest for comparison with calculation data. In this case the detector count is mainly determined by scattering by air in the channel, and it is many orders of magnitude higher than the expected one for the case of vacuum channel. To test the under-reactor shielding, measurements of fast neutron flux density are of most interest. These measurements have been performed, but the analysis cannot be completed until the calibration measurements of the efficiency of the fast neutron detector used are made. In the near future it is planned to carry them out.

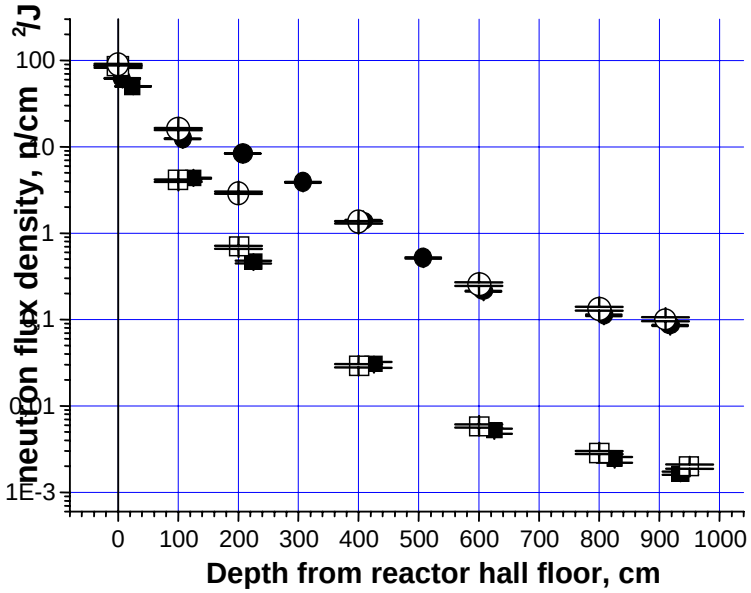

Fig.6. *Thermal neutron flux densities at 1 J in the under-reactor shaft depending on its depth. Full circles (squares) – measurement data, open circles (squares) – calculation data. Circles and squares correspond to different geometries of the collimator.*

The "back" (opposite to the detector) flight base of the neutron channel of the experimental setup has been manufactured. Vacuum tests of this part of the channel have been carried out. Then the whole inner surface has been covered with cadmium 1 mm thick and vacuum tests have been repeated. The "back" flight base has been transported to Snezhinsk.

The manufacturing and installation of the whole experimental setup, as well as equipment operation tests are scheduled for 2005.

1.6.4. Search for new interactions of neutrons with nuclei

From the analysis of experimental neutron scattering data the constraints for the interaction constant of the Yukawa potential as a hypothetical correction to the Newtonian gravitational potential, have been obtained. The constraints have been determined for the interaction radius in the range between 10^{-2} and 10^{-7} cm, where experiments to measure the Casimir forces by atomic-force microscopy are not sensitive. Also, experimental limitations for non-electromagnetic neutron-nucleus potentials of the power-law type have been obtained. Several possibilities to strengthen the limitations have been discussed.

1.7. Ultracold neutron physics, neutron optics

1.7.1. Diffraction from a moving grating as a non-stationary quantum effect

At the UCN source in ILL (Grenoble, France) a new experiment to obtain UCN spectra of diffraction by a moving grating has been carried out. In contrast to the first demonstration experiment, the new one allows a quantitative comparison with the theory to be made. As in the previous case, the initial beam monochromatization, as well as the analysis of the spectra have been performed with the help of the Fabry-Perot (FP) interferometers. The device used was the gravitational spectrometer with FP interferometers. In the experiment the energy quantization effect has been reliably observed, which is a result of the phase modulation of a neutron wave due to a phase grating that moves across. The obtained spectrum splitting determined by the modulation frequency coincides with the calculated value within 2% error, and the diffraction efficiency of the grating (wave intensity of the first order) is 38%, which is close to the maximum limiting value for this type of gratings. The invariability of the spectral line width when the grating rotates allows one to obtain low estimates for cross-sectional sizes of the incident flat wave front. This cross-sectional coherent length is no less than 0.07 cm, which is 1000 times greater than the neutron wavelength (**Fig.7**).

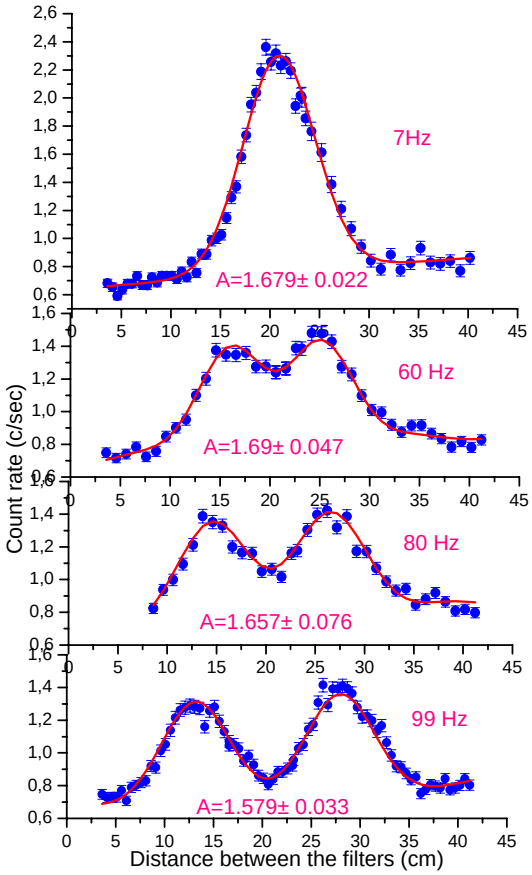

Fig.7*. Transformation of the UCN spectrum when neutrons pass through the rotating grating. The rotation frequency is given in the graphs.*

The rotating grating with the spatial period α depending on its azimuth angle was used to actively influence the energy and velocity of neutrons to focus neutrons in time. During the first half of the grating revolution the neutrons with an energy $E(t) = \hbar[\omega - \Omega(t)]$ (where $\Omega = 2\pi f \alpha^{-1}$ is the modulation frequency, f is the grating rotation frequency) satisfy the condition of the focusing. During the second half of the grating revolution the neutrons with an energy $E(t) = \hbar[\omega + \Omega(t)]$ meet

the condition of the focusing. As a result, the neutrons coming into the setup in arbitrary moments achieve the detector grouping around a specific time moment - point of the time focusing. The efficiency of such focusing obtained to date is about 28% (**Fig. 8**).

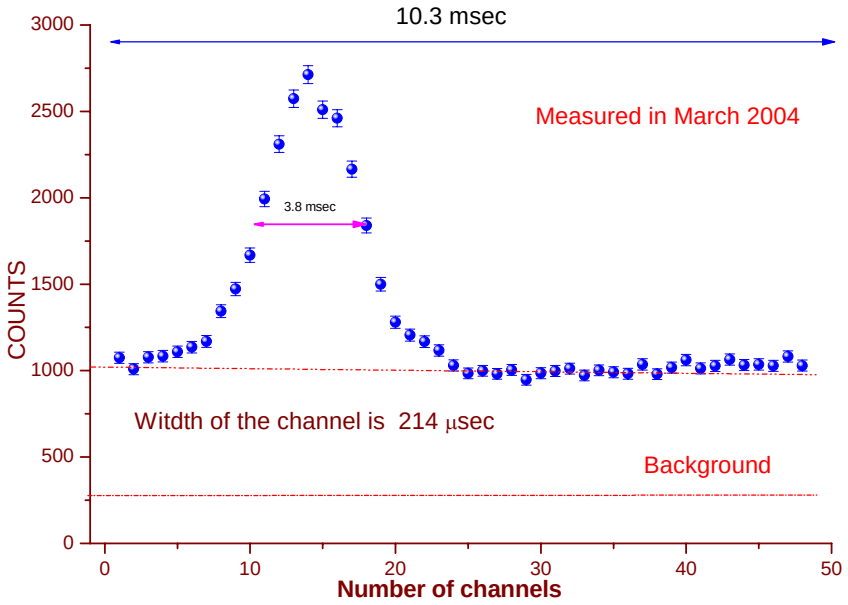

***Fig.8**. Time focusing peak.*

1.7.2. Quantum effects in one-dimensional gravity-magnetic trap

The problem of ultracold neutron storage above a plane magnetic Vladimirsky mirror in the presence of gravitation has been solved. For neutrons with defined polarization the total (magnetic and gravitation) potential can have a minimum, forming a gravity-magnetic trap**.** At small energies of vertical motion, the neutron state in such a well appears to be quantized. At quite realistic values of the magnetic mirror parameters the wave functions of the first several states are localized in a region of several tens of microns. The location of the localization region is sensitive to the magnitude of the free fall acceleration of the neutron.

1.7.3. Investigations of the neutron lifetime and anomalous losses in UCN storage

Throughout the past year a new UCN trap of monocrystalline sapphire of 30 cm in length and 3.6 cm in diameter has been designed and a new setup making it possible to measure the time of UCN storage in the trap in a temperature range from 80 to 800 K has been constructed. Measurements with the UCN source in ILL (Grenoble, France) have been made. The program of the measurements has been fulfilled completely. The best value of the loss factor obtained with this setup is an order of magnitude greater than that predicted by the theory. To understand the reason of this disagreement additional investigations are required.

The measurements (in collaboration with PNPI and ILL) of the neutron life time with an accuracy better than 1 s: $878.5 \pm 0.7 \pm 0.3$ s have been made. This result differs from the mean world value by six standard deviations. However, the new value of the neutron lifetime together with the asymmetry in the electron escape is in good agreement with the Standard model.

1.7.4. Investigations to design cold neutron sources

The experiment (in collaboration with PSI and ILL) on direct measurements of the UCN generation in gas, liquid and solid deuterium in a temperature range from 80 to 800 K has been carried out. The obtained result is in agreement with the calculations in incoherent approximation. The detailed calculations of the UCN generation and energy release in moderators at the "TRIGA" pulsed reactor have been performed. A number of measurements of the heat release in various materials and the comparison with the calculations have been carried out. A simple method to calculate the transport of ultra slow neutrons in a cold moderator with a fast change in temperature has been suggested and used. Also, the neutron transport in granular medium has been considered. The calculations can be used to optimize moderators of ultracold and very cold neutrons at pulsed sources.

2. Theoretical investigations

2.1. Theoretical investigations of neutron β-decay

The current level of investigations in the physics of electroweak interactions requires reliable knowledge of characteristics of the neutron β-decay with an accuracy of ~0.1 %. In this connection, in 2004 the investigations to achieve the best precision in the determination of radioactive corrections in the neutron decay were performed.

For correct calculations of the radioactive corrections the calibration invariant interaction of nucleons with the electromagnetic field is included on the basis of the model of vector domination. The nucleon structure is effectively taken into account in this approach due to the fact that along with the direct interaction of electromagnetic field with isovectorial and isoscalar nucleon current, the calibration invariant interaction of the electromagnetic field with nucleons through vectorial β-, φ-, ω-mesons is included as well. Such consideration of the nucleon structure in the frame of the model of vectorial domination results in the form-factors of type $-m_\rho^2/(k^2 - m_\rho^2)$ in all electromagnetic vertices, as well as in additional contributions in the radioactive corrections providing the calibration invariance in the calculations of the corrections.

The nucleon structure is also taken into account by means of algebra of currents. When calculating the radioactive corrections it is possible to connect the nucleon propagation function with electroweak nucleon vertices in a general form taking into account strong interactions.

The performed work allows one to reliably judge about the magnitude of the radioactive corrections with an accuracy of ~0.1%, which is required for further refinements of characteristics of electroweak interactions from the treatment of experimental data.

2.2. Theoretical investigations of pair correlation functions of fission neutrons

Theoretical investigations of pair correlation functions of neutrons with small relative momentum ($0 \leq |\mathbf{q}| \leq 100$ MeV/c) formed in the process of fission of heavy atomic nuclei ($A \geq 200$) have been performed. The general method of pair momentum correlation of particles with small relative momentum in the frame of the model of point one-particle sources has been used. In a general case the pair correlation of neutrons is determined both by the effect of the Fermi statistics and the S-wave strong interaction in the final state (the latter takes place only for a singlet state of the neutron pair). It has been found that for usual fission neutrons (escaped from fragments) the pair correlation at non-zero relative momentum is practically absent due to a great difference in emission times ($> 10^{-19}$ s), and two-neutron correlation function is sensitive to the effects of interaction in the final state only for pairs of instant ("pre-scission" and "scission") neutrons (corresponding emission times of the order of 10^{-21} - 10^{-22} s, sizes of emission region of the order of several Fm). Thus, the correlation method in principle can be applied to determine a share of pairs of instant ("pre-scission" and "scission") neutrons in the total number of neutron pairs fixed in the fission.

Applied research. In 2004 work to study atmospheric deposition of heavy metals by means of biomonitoring, NAA and GIS technologies (REGATA Project) over the territory of Central Russia (Tulskaia, Tverskaia, Yaroslavskai reagions and south-east of Moskovskaia region) as well as in Armenia (Sevan) and Vietnam, continued. Organizational and methodological work to get ready for the next European simultaneous collection of moss-biomonitors of heavy metal atmospheric deposition (moss-survey) to be held in 2005 in a number of JINR member and non-member states (Belorussia, Ukraine, Bulgaria, Bosnia, Macedonia, Poland, Romania, Serbia, Slovakia, Turkey (European part)) has been done.

A comparative analysis of various biomonitors (lichens, tree bark) and of soils from the region of the oil-refining plant in Constance, Romania has been carried out. The possibility of using biomonitors for the assessment of the influence of the plant on the natural environment of the recreational area on the Black Sea coast of Romania has been demonstrated.

Neutron activation analysis of over 250 samples of vegetation and animal origin has been conducted under the Coordination Program (2002-2005) and the Project for Technical Cooperation with IAEA (2003-2005) for supervision and quality of food products grown in the conditions of strong antropogenic pollution.

In 2004 the final stage of work under the project «Monitoring of working places and occupational health of personnel engaged in production of phosphate fertilizers at plants in Russia, Uzbekistan, Poland and Romania» (European Program 5, Copernicus) was completed. The results of analysis of ecological samples (raw materials, soils, sediments, water and air filters) and of human biosubstrates (hair, nails, urine and teeth) have been presented at two international conferences and are submitted for publication.

Work to develop new pharmaceuticals and sorbents on the basis of the blue-green alga *Spirulina platensis* in cooperation with a group of biophysicists in the Institute of Physics of the Georgian Academy of Sciences continued. Part of the investigations was conducted at the reactor of the University of Texas, USA. In 2004 the patent for the method of the production of the *Spirulina* biomass containing chrome was granted.

The analysis of the data from the study of the effect of neutrons lying in the fission spectrum on the physical properties fine-crystal diamonds obtained in the Institute of Physics of Solid Matter and Semiconductors of the National Academy of Sciences of Belorussia (Minsk) has been completed.

1. НАУЧНЫЕ ИССЛЕДОВАНИЯ

1.1. ФИЗИКА КОНДЕНСИРОВАННОГО СОСТОЯНИЯ

Главные научные результаты

Дифракция. С помощью совместного анализа рентгеновских и нейтронных (полученных на ФДВР) дифракционных данных была решена кристаллическая структура однофазного соединения Li_2BeD_4. Соединение кристаллизуется в моноклинной сингонии (пространственная группа $P2_1/c$) с параметрами решетки $a = 7.06228(9)$ Å, $b = 8.3378(1)$ Å, $c = 8.3465(1)$ Å, $\beta = 93.577(1)°$, $Z = 8$. Его структура содержит изолированные тетраэдры BeD_4 и атомы Li в между ними (**Рис.1**) и сохраняется без каких либо заметных изменений вплоть до 8 K. Определение кристаллической структуры Li_2BeD_4 является первым реальным результатом для тройных гидридов в системе Li-Be-H. Оно продемонстрировало мощь современных структурных вычислительных программ для прямого определения структуры из порошковых дифракционных спектров и преимущества одновременного использования нейтронных и рентгеновских данных для получения структурной информации о системах, состоящих из самых легких атомов.

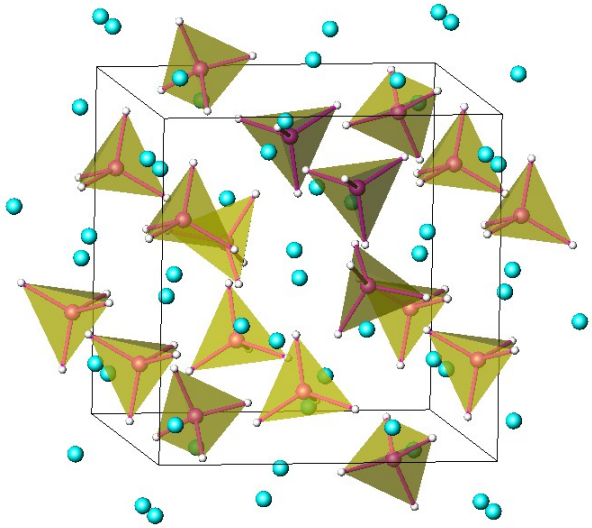

Рис.1. *Кристаллическая структура соединения Li_2BeD_4, восстановленная по данным нейтронной дифракции*

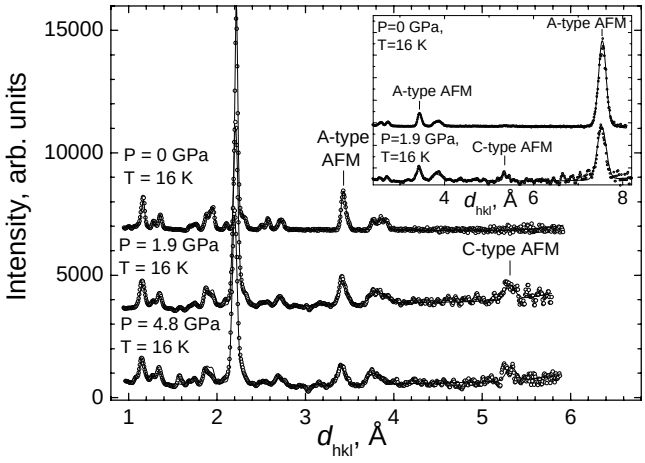

Рис.2. *Участки нейтронных дифракционных спектров $Pr_{0.44}Sr_{0.56}MnO_3$, измеренных при высоких давлениях $P = 0$, 1.9 и 4.8 ГПа, $T = 16$ K и обработанных по методу Ритвельда. С повышением давления наблюдалось появление новой АФМ фазы С-типа.*

На дифрактометре ДН-12 проведено исследование влияния высокого давления до 5 ГПа и низкой температуры в диапазоне 15 – 300 К на атомную и магнитную структуру манганитов $Pr_{1-x}Sr_xMnO_3$ (x = 0.5, 0.56). Соединения $Pr_{0.44}Sr_{0.56}MnO_3$ и $Pr_{0.5}Sr_{0.5}MnO_3$ при нормальном давлении имеют тетрагональную структуру (пр. гр. I4/mcm). С понижением температуры в $Pr_{0.44}Sr_{0.56}MnO_3$ наблюдается фазовый переход в антиферромагнитную (АФМ) фазу А-типа (**Рис.2**), который сопровождается структурным фазовым переходом из тетрагональной в орторомбическую структуру (пр. гр. Fmmm). В $Pr_{0.5}Sr_{0.5}MnO_3$ с понижением температуры наблюдаются переходы в промежуточную тетрагональную ФМ фазу и низкотемпературную орторомбическую АФМ фазу А-типа. При высоком давлении $P \approx 2$ ГПА в $Pr_{0.44}Sr_{0.56}MnO_3$ возникает новая тетрагональная АФМ фаза С-типа, которая сосуществует с исходной орторомбической фазой А-типа в области низких температур. В $Pr_{0.5}Sr_{0.5}MnO_3$ влияние высокого давления приводит к значительному возрастанию температуры фазового перехода из тетрагональной ФМ фазы в орторомбическую АФМ фазу А-типа. В области низких температур наблюдается сосуществование исходной орторомбической АФМ фазы А-типа с тетрагональной фазой, не проявляющей признаков наличия дальнего магнитного порядка.

Научная программа на дифрактометрах EPSILON и SKAT была сконцентрирована на: исследовании внутренних напряжений в поликристаллических материалах (в основном в горных породах), текстурном анализе геологических материалов и определении анизотропных физических свойств горных пород по кристаллографическим текстурам. В частности, проведены исследования остаточных напряжений строительных материалов из мрамора, направленные на лучшее понимание процессов, ведущих к деформации конструкций.

Впервые методами нейтронной дифрактометрии и акустической эмиссии (АЭ) исследована динамика α-β-перехода в образце природной горной породы – кварците. Измерены изменения межплоскостных расстояний кристаллической решетки в процессе α-β-перехода (**Рис.3**) и на этой основе оценены значения внутренних напряжений (**Табл.1**), которые в несколько раз превысили приложенное к образцу внешнее механическое напряжение. Установлено, что после завершения α-β-перехода возникали вспышки АЭ, превышающие на два порядка по интенсивности уровень АЭ, обусловленный термическим растрескиванием при нагревании образца. Возникновение вспышек упругих колебаний АЭ при фазовом переходе в породообразующем минерале земной коры – кварце свидетельствует о дискретном характере неустойчивости. Не исключено, что такие явления могут способствовать развитию очага землетрясения за счет изменения напряженного состояния среды или триггерного эффекта.

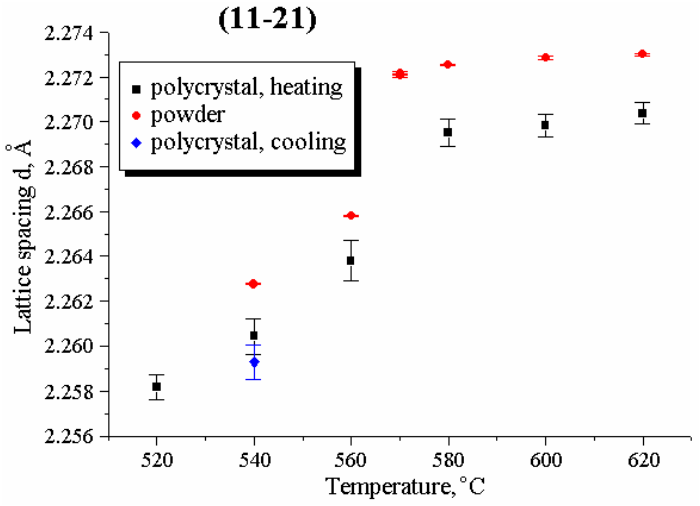

Рис.3. *Температурная зависимость межплоскостного расстояния (11-21) в порошке кварца и поликристалле (нагрев и охлаждение)*

Таблица 1

Внутренние микро- ($\sigma_{LATTICE}$) и макро- (σ_{MACRO}) напряжения в кварците в области α – β перехода.

(*hkil*)	T, °C	Δd/d, $*10^{-3}$	Модуль Юнга E, GPa	$\sigma_{LATTICE}$, MPa	σ_{MACRO}, MPa
$(10\bar{1}0)$	540	1.24	76.3 84.0	94.6 104.2	-25
	600	0.03	116.4 110.7	3.5 3.3	-27
$(11\bar{2}1)$	540	1.00	76.3 84.0	76.3 84.0	-25
	600	0.14	116.4 110.7	16.3 15.5	-27

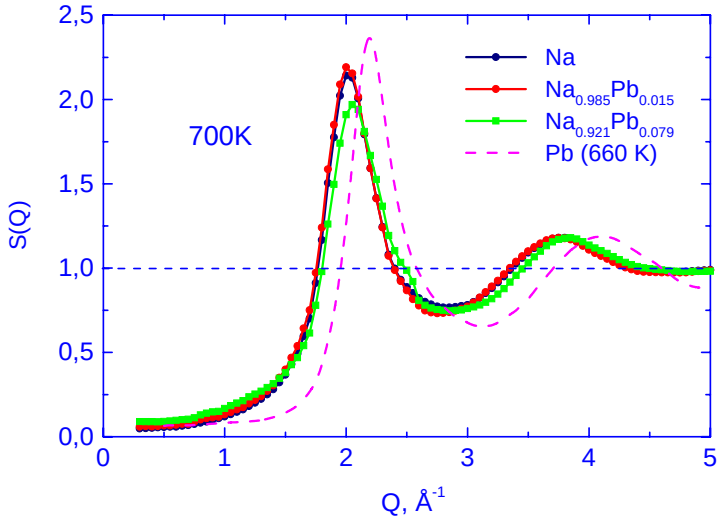

Рис.4*. Структурные факторы жидкого натрия и расплавов Na–Pb.*

Неупругое рассеяние. На спектрометре неупрого рассеяния ДИН-2ПИ проведено сравнение экспериментальных данных по системе натрий-свинец (**Рис.4**) с расчетом на основе моделирования методами молекулярной динамики. Сделан вывод о том, что при низких концентрациях примеси C_{Pb} ~10 % ат. и менее кластеры типа Na_4Pb в заметном количестве отсутствуют, и растворенный свинец присутствует в расплаве в атомарном состоянии. Такой вывод позволяет более осознанно подходить к оценкам термодинамических и физико-химических свойств этого расплава.

На спектрометре НЕРА-ПР выполнены эксперименты и проведено моделирование функции плотности колебательных состояний в твердом метаноле, дейтерированном различным образом: CH_3OH, CH_3OD, CD_3OH, CD_3OD (**Рис.5**). Показано, что метанол может эффективно использоваться как стандарт для оценки качества компьютерной симуляции динамики молекул в кристаллической и аморфных фазах.

Рефлектометрия поляризованных нейтронов. На рефлектометре с поляризованными нейтронами РЕМУР исследовалось явление сверхпроводимости и магнетизма на границе раздела сверхпроводника с ферромагнетиком. В частности, были исследованы слоистые структуры, в которых одновременно существуют составленные из сверхпроводящих слоёв ванадия и ферромагнитных слоёв железа периодические структуры Fe/V плюс бислои V/Fe и $V/Fe_{0.66}V_{0.34}$ (**Рис.6**). Показано, что эффекты влияния

сверхпроводимости на магнетизм сильно зависят от состава и структуры магнитного слоя. Полученный результат является принципиально новым для слоистых структур.

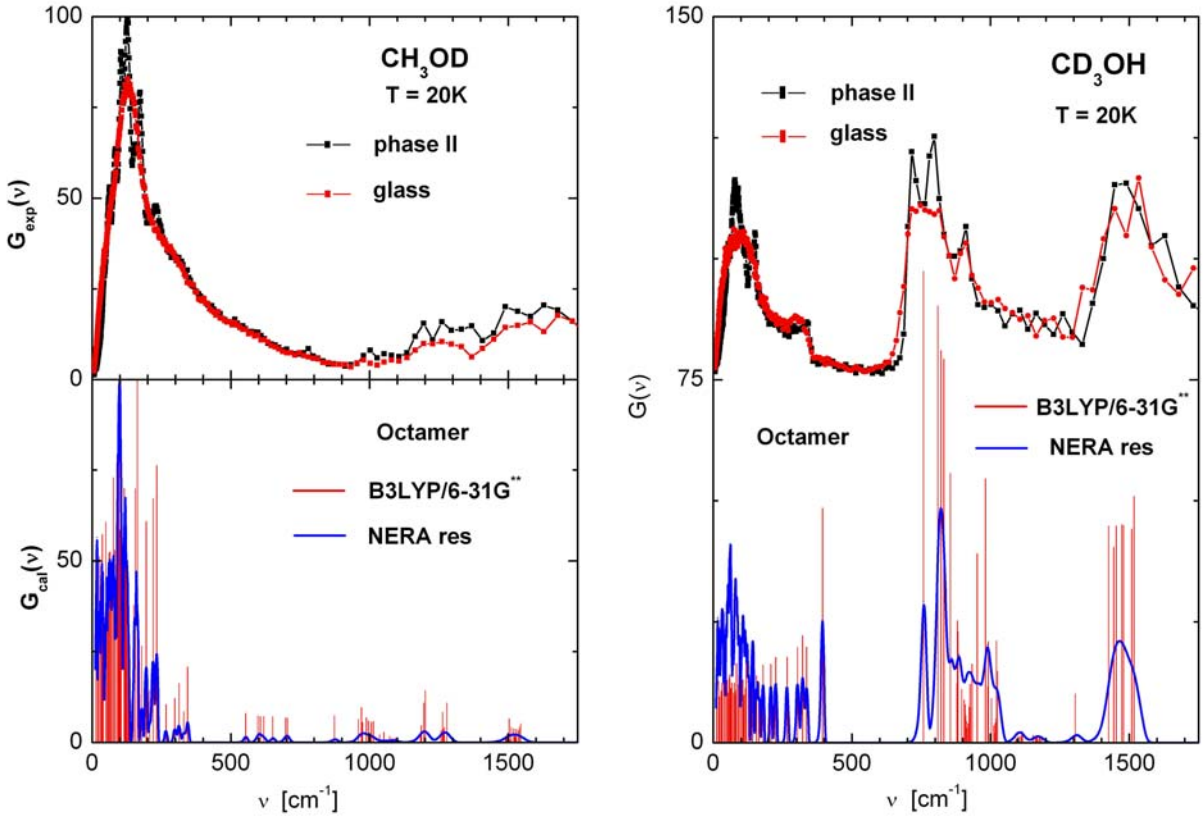

Рис. 5. *Изотопный и структурный эффекты на колебательный спектр метанола.*

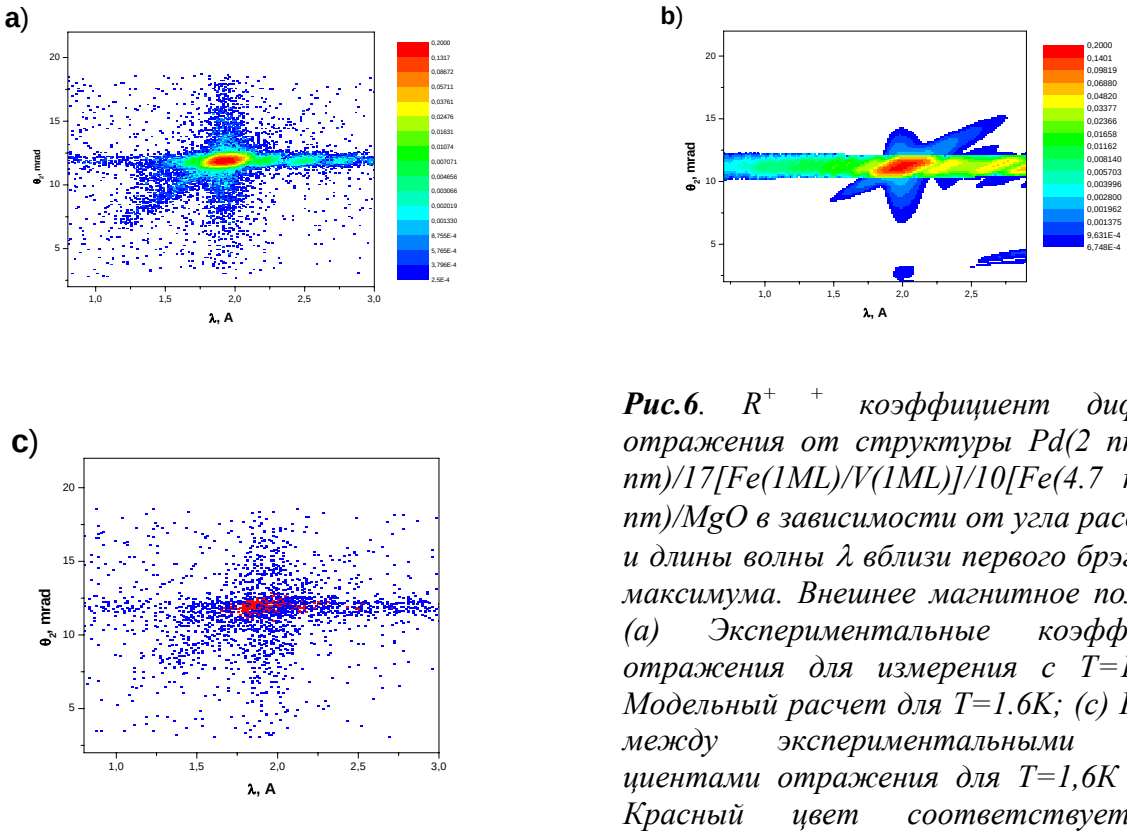

Рис.6. *$R^{+}{}^{+}$ коэффициент диффузного отражения от структуры Pd(2 nm)/V(36.5 nm)/17[Fe(1ML)/V(1ML)]/10[Fe(4.7 nm)/V(4.7 nm)/MgO в зависимости от угла рассеяния θ_2 и длины волны λ вблизи первого брэгговского максимума. Внешнее магнитное поле 0.7кЭ. (a) Экспериментальные коэффициенты отражения для измерения с T=1.6K; (b) Модельный расчет для T=1.6K; (c) Разность между экспериментальными коэффициентами отражения для T=1,6K и T=7K. Красный цвет соответствует положительной величине, синий – отрицательной.*

Малоугловое рассеяние нейтронов. На установке малоуглового рассеяния нейтронов ЮМО проведены исследования ряда полимерных систем, дендримеров, а также смешанных растворов полимеров и поверхностно-активных веществ. При изучении структуры поликарбосилановых дендримеров с различным молекулярным строением были выявлены структурные особенности укладки концевых групп дендримеров, а именно их слоистый характер. Это, по-видимому, является причиной ограничения роста дендримеров при увеличении степени генерации.

Проведены эксперименты по малоугловому рассеянию нейтронов на высокостабильных магнитных жидкостях с водной основой. Получены параметры коллоидных частиц жидкостей при различных концентрациях диспергированного магнитного вещества (магнетит) (**Рис.7**). Проведено сравнение структуры данных жидкостей с менее стабильными водными образцами, использующие другие ПАВ для стабилизации, а также с высокостабильными магнитными жидкостями на основе неполярных носителей, таких как бензол.

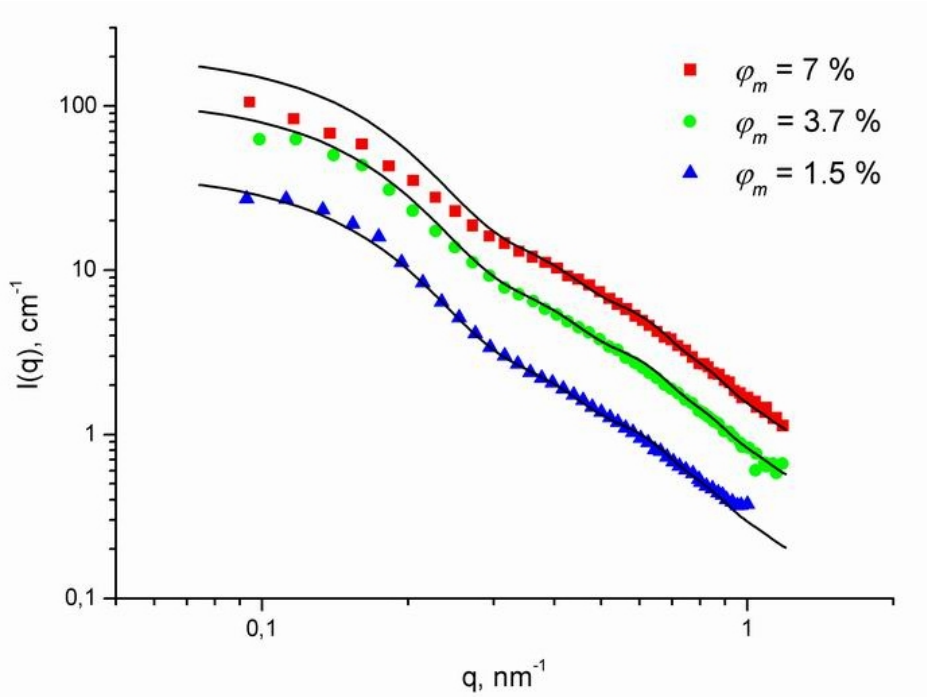

Рис.7*. Экспериментальные данные (точки) малоуглового рассеяния на магнитной жидкости Fe_3O_4/DBS+DBS/D_2O при различной объемной доли магнитного материала, φ_m. Магнетит получен с помощью химической конденсации. Стабильность системы осуществляется посредством двойного слоя додецилбензолсульфоновой кислоты. Линии отвечают расчетным кривым согласно модели «ядро-оболочка» для невзаимодействующих частиц. Эффект взаимодействия не проявляется вплоть до φ_m=4 %. Отклонение верхней экспериментальной кривой от модельной при малых значениях q отражает «мягкое» взаимодействие между коллоидными частицами.*

Исследована коагуляция водных дисперсий фуллеренов при добавлении в них различных солей. При этом анализировалась временная эволюция спектров поглощения видимого и ультрафиолетового излучения. Обнаружено, что концентрация фуллеренов в растворах монотонно уменьшается после добавления соли, что подтверждает зарядовую природу стабилизации колллоидных частиц в данных системах. Измеренные пороги коагуляции значительно отличаются от доложенных ранее. Проведены эксперименты и предварительная обработка данных по малоугловому рассеянию нейтронов на коагулирующих водных растворах фуллеренов в режиме реального времени. Получены оценки динамика роста кластеров фуллеренов и их концентрации в растворе при коагуляции.

Методом нейтронной дифракции проведены исследования структуры модельных мембран Stratum Corneum. Исследована структура смешанной четырехкомпонентной системы церамид 6/холестерин/пальмитиловая кислота/сульфат холестерина с различными весовым соотношениями компонент и низким уровнем гидратации. Определено положение холестерина в липидном бислое. Измерена функция распределения воды в бислое. Доказано, что модельные мембраны Stratum Corneum имеют малую гидратацию межмембранного пространства по сравнению с фосфолипидами.

Главные методические результаты

Проведена модернизация рефлектометра РЕМУР на импульсном реакторе ИБР-2. В результате, в несколько раз был снижен радиационный фон на спектрометре, а также повысилась интенсивность пучка нейтронов, прошедшего многоканальный поляризатор. В спектрометре реализована конструкция из двух зеркал-поляризаторов, что позволило значительно увеличить поляризацию пучка нейтронов. Разработано новое программное обеспечение спектрометра, основанное на использовании VME-PSI адаптера, что повысило надёжность работы.

Проведена модернизация рефлектометра РЕФЛЕКС. Тестовые измерения на установке в сентябре-октябре 2004 г. показали, что в результате переноса механического прерывателя рабочая часть спектра тепловых нейтронов увеличилась с $\Delta\lambda$=5Å до 10Å, что значительно расширило диапазон регистрируемых значений переданного импульса рассеянных нейтронов.

На спектрометре ДИН-2ПИ в соответствии с планом завершено проектирование нового корпуса термостата TS-3000M. Разработаны рабочие чертежи на изготовление модернизированного варианта обечайки корпуса термостата. Реконструирован блок радиационных экранов. Использование новых материалов, в частности, более технологичных (по сравнению с чистым вольфрамом) вольфрам-рениевых сплавов, позволило создать конструкцию блока, более удобную при варьировании количества экранов, их материала и толщины в зависимости от параметров эксперимента.

На рефлектометре РЕМУР разработан алгоритм применения различных теоретических подходов для расчета диффузного рассеяния в эксперименте по рефлектометрии нейтронов. Созданы пакеты компьютерных программ для модельных расчетов и фитирования экспериментальных данных рассеяния нейтронов от магнитных многослойных наноструктур. Выполненная работа позволяет проводить более корректную обработку экспериментальных данных рассеяния поляризованных нейтронов от магнитных многослойных наноструктур и исследовать эффекты близости на масштабах $1 \div 10^4$ нм.

В группе биофизических исследований на основе гидрофобно-гидрофильной модели бислоя с линейной функцией распределения воды и модели разделенных форм факторов разработано программное обеспечение для описания внутренней структуры мембраны липидных везикул по спектрам малоуглового рассеяния нейтронов и проведены исследования нескольких липидных систем методом малоуглового рассеяния нейтронов.

1.2. НЕЙТРОННАЯ ЯДЕРНАЯ ФИЗИКА

Введение

В течение 2004 основные работы в области нейтронной ядерной физики в ЛНФ им. И.М. Франка проводились на установке ЭГ-5, на нейтронных пучках других ядерных центров России, Болгарии, Польши, Чехии, Германии, Республики Корея, Китая, Франции, США и Японии. Исследования проводились по традиционным направлениям: изучение процессов нарушения пространственной и временной четности при взаимодействии нейтронов с ядрами; изучение квантово-механических характеристик, энергетики и динамики процесса деления; экспериментальное и теоретическое исследование электромагнитных свойств нейтрона и его бета-распада; гамма-спектроскопия нейтронно-ядерных взаимодействий; структура атомного ядра; получение новых данных для реакторных приложений и для ядерной астрофизики; эксперименты с ультрахолодными нейтронами; прикладные исследования.

1. Экспериментальные исследования

1.1. Нарушение пространственной и временной четности при взаимодействии нейтронов с ядрами

1.1.1 Поиск и исследование структуры подпороговых нейтронных p-резонансов на изотопах свинца методом комбинированной корреляционной гамма-спектроскопии

В течение года был завершён анализ экспериментальных результатов проведенных в 2002 – 2003 г.г. экспериментов по поиску отрицательного нейтронного p-резонанса у изотопов свинца с целью объяснения обнаруженного ранее эффекта нарушения пространственной чётности, проявившемся во вращении спина поляризованных тепловых нейтронов при прохождении их через образец. В связи с необходимостью дополнительной проверки полученных результатов, свидетельствующих о наличии сильного p-волнового резонанса у изотопа ^{207}Pb, а не у ^{204}Pb, как ожидалось на основании данных предшествующих работ группы ИТЭФ, проводилась подготовка к реконструкции гамма-спектрометра COCOS с целью увеличения его эффективности и быстродействия.

1.1.2 Подготовка к исследованию T-неинвариантных эффектов в нейтронно-ядерных взаимодействиях

Продолжалось развитие методики измерения T-неинвариантных эффектов в нейтрон-ядерных взаимодействиях. Наиболее перспективными в настоящее время считаются измерения трёхвекторной P-нечётной T-нечётной и пятивекторной P-четной T-нечётной корреляций векторов **I**, **k**, **s**. При исследовании пятивекторной корреляции необходима выстроенная, неполяризованная мишень с ядрами, обладающими p-резонансами в энергетической области до 100 эВ. При исследовании трёхвекторной корреляции необходима поляризованная ядерная мишень с p-резонансами, в которых наблюдался P-нечётный эффект. Проводить такого рода эксперименты необходимо на интенсивных источниках нейтронов. В связи с изложенным, работа в данной области велась по двум направлениям:
I. Для исследования пятивекторной корреляции выстроенная ядерная мишень может быть получена статическим методом, использующим квадрупольное взаимодействие ядер с кристаллическим полем при низких температурах, или, возможно, с использованием недавно предложенного метода динамического выстраивания ядер. Для статического метода были проведены оценки величины выстроенности ядер йода-127 в монокристалле йода при низких

температурах. Было выяснено, что пригодная для измерений выстроенность ~50% может быть получена при охлаждении монокристалла йода до температуры ~20-50 мК. Для проверки идеи динамического выстраивания ядер было проделано следующее:

- Совместно с ИТЭФ был приготовлен монокристалл ниобата лютеция с парамагнитной примесью.
- Проведены измерения ЭПР-спектров этого кристалла.
- Проведен пробный сеанс динамического выстраивания, который показал необходимость создания более чувствительного, широкодиапазонного Q-метра, неразрушающего выстроенность.
- В настоящее время ведутся работы по созданию такого Q-метра.

II. Для исследования трёхвекторной корреляции наиболее перспективной считается поляризованная лантановая мишень, поскольку в p-волновом резонансе ^{139}La при энергии 0.75 эВ наблюдался большой P-нечётный эффект. Создание соответствующей поляризованной мишени с использованием монокристалла $LaAlO_3$:Nd+ предполагается осуществлять в сотрудничестве с КЕК (Япония). В настоящее время группа располагает монокристаллическим образцом $LaAlO_3$, предоставленным японской стороной, для проведения экспериментов по получению поляризованной мишени. Уже проведены нейтронографические исследования кристаллической структуры этого образца, которые показали его пригодность для проведения пробных экспериментов по динамической поляризации ядер ^{139}La.

1.1.3 Статус проекта KaTRIn

В рамках сотрудничества с КЕК (Япония) была модифицирована установка для измерения поляризации ^{3}He методом пропускания нейтронов. Модификация была предпринята с целью измерения псевдомагнетизма поляризованных ядер ^{129}Xe и ^{131}Xe. Схема модифицированной установки показана на **рис. 1.**

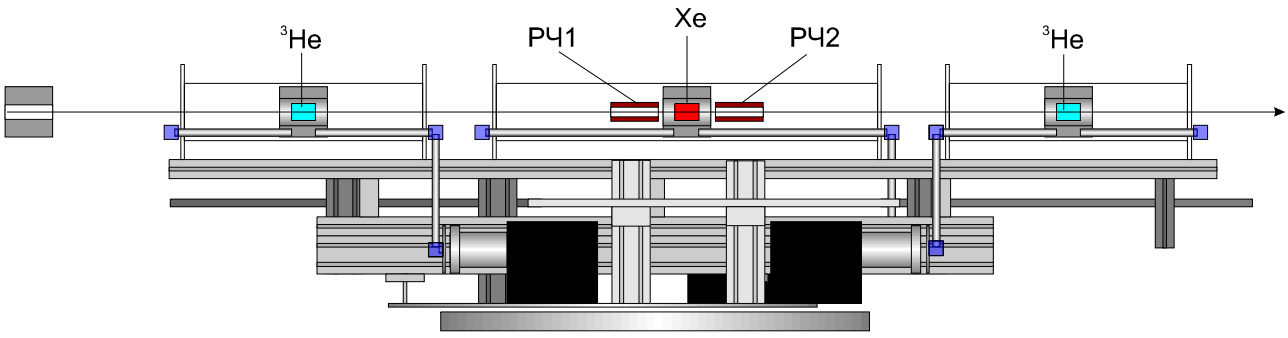

Рис. 1. *Схема экспериментальной установки.*

На рисунке нейтронный пучок направлен слева направо. Левая ячейка с поляризованным ^{3}He выполняет роль поляризатора нейтронов. После прохождения ячейки нейтроны поляризованы вдоль направления пучка. Радиочастотная катушка РЧ1 поворачивает поляризацию нейтронов относительно вертикальной оси так, что на входе в ячейку с поляризованным Xe (естественная смесь изотопов), она перпендикулярна плоскости рисунка. Радиочастотная катушка РЧ2 поворачивает нейтронную поляризацию обратно к направлению пучка, а правая ячейка с поляризованным ^{3}He выполняет роль анализатора поляризации.

Псевдомагнитное взаимодействие поляризованных нейтронов с поляризованными ядрами Xe должно приводить к вращению плоскости поляризации пучка. В этом случае экспериментальный эффект должен проявиться в виде разности отсчетов детектора для

измерений с поляризованным и неполяризованным Xe. На практике предполагается измерять разность трансмиссий поляризованного нейтронного пучка в области 0.02 - 0.1 эВ.

^{3}He и нечетные изотопы Xe поляризуются методом оптической накачки (оптические части установки на рисунке не показаны).

В настоящее время проводится тестирование установки на нейтронном пучке.

1.1.4 Создание поляризованной протонной мишени

Изготовлены и испытаны непрерывные и дискретные серебряные теплообменники криостата растворения ^{3}He в ^{4}He со сверхпроводящим соленоидом. Криостат предназначен для поляризации ядер методом "грубой силы" и динамической накачкой поляризации. Собран тракт растворения ^{3}He в ^{4}He, завершено испытание и определены параметры криостата. Результаты испытания:

- минимальная температура на образце T= 24 мK;
- скорость циркуляции n= 0.98 ммоль/сек;
- напряженность магнитного поля в центре соленоида H= 5.8 T при однородности магнитного поля $\Delta H/H = 10^{-4}$.

Для поляризованной протонной мишени изготовлены пластинки гидрида титана TiH_2 диаметром 14 мм и толщиной 0.2 мм, полученные с помощью прессовки порошка гидрида титана под давлением $2\cdot10^6$ г/см^2. На пучке №1 ИБР-2, на спектрометре поляризованных нейтронов завершаются работы по монтажу установки поляризованной ядерной мишени.

1.2 Нейтронно-индуцированное и спонтанное деление

1.2.1 Исследование тройного деления ^{235}U на пучке холодных нейтронов в ИЛЛ (Гренобль)

В 2004 году на пучке ПФ-1 реактора ИЛЛ в Гренобле (Франция) был проведен эксперимент по исследованию тройного нейтронно-индуцированного деления ^{235}U. Эксперимент проводился в коллаборации с учеными из лаборатории ядерных реакций, ПИЯФ (Гатчина), Германии и Франции. Эксперимент явился продолжением серии работ по исследованию процесса тройного деления, которые проводились на спонтанных источниках ^{252}Cf. Целью данной работы являлось изучение массово-энергетических корреляций осколков деления и легких заряженных частиц для более легкой делящейся системы, которой является ^{236}U*.

Осколки деления измерялись быстрой двойной ионизационной камерой с секторированным катодом, позволяющим определять энергии, массы, а также направления вылета осколков деления, а для регистрации легких заряженных частиц использовались ΔE-E телескопы высокого разрешения, позволяющие идентифицировать частицы по заряду и массе от изотопов водорода до бериллия, а также измерять их энергии и угловые распределения. В течение 20 дней пучкового времени было накоплено около 4×10^7 событий с испусканием α-частиц, 3×10^5 событий с ^{6}He, 1×10^4 с изотопами Li и 6×10^3 с изотопами Be.

В результате были получены предварительные данные по выходам, энергетическим и угловым распределениям легких заряженных частиц, получены массовые и энергетические распределения осколков деления для различных мод тройного деления. Данный эксперимент позволяет также исследовать некоторые свойства четверного деления с одновременным вылетом двух α-частиц или α-частицы и трития. Пример энергетических распределений осколков деления для двух мод четверного деления представлен на **рис. 2**.

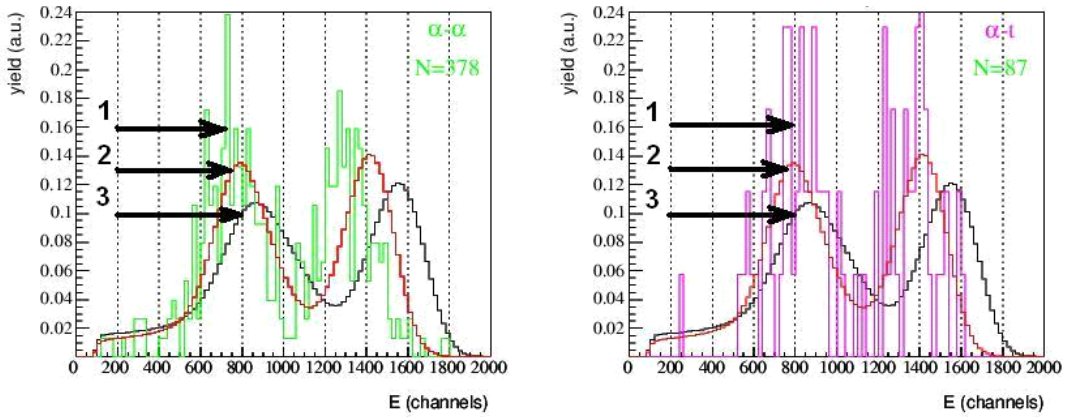

***Рис. 2**. Энергетические распределения осколков деления (сырые данные) для четверного деления $^{235}U(n_{th},f)$ с вылетом двух α-частиц (слева) и α-частицы и трития (справа) – гистограмма 1. Гистограмма 2 соответствует тройному деления с вылетом α-частицы, гистограмма 3 – двойному делению.*

1.2.2 Исследование нейтрон-нейтронных корреляций в спонтанном делении ^{252}Cf

В рамках подготовки к эксперименту по изучению вылета нейтронов в тройном делении ^{252}Cf, а также по поиску предразрывных нейтронов (scission neutrons) и изучению нейтрон-нейтронных корреляций был проведен тестовый эксперимент с использованием многосекционного нейтронного детектора DEMON в Страсбурге (Франция). В эксперименте использовался спектрометрический источник ^{252}Cf на тонкой никелевой подложке, помещенный в двойную ионизационную камеру, позволяющую определять энергии, массы и направления вылета осколков деления. Нейтроны деления регистрировались нейтронными детекторами DEMON, расположенными под различными углами к оси камеры деления (см. **рис. 3**).

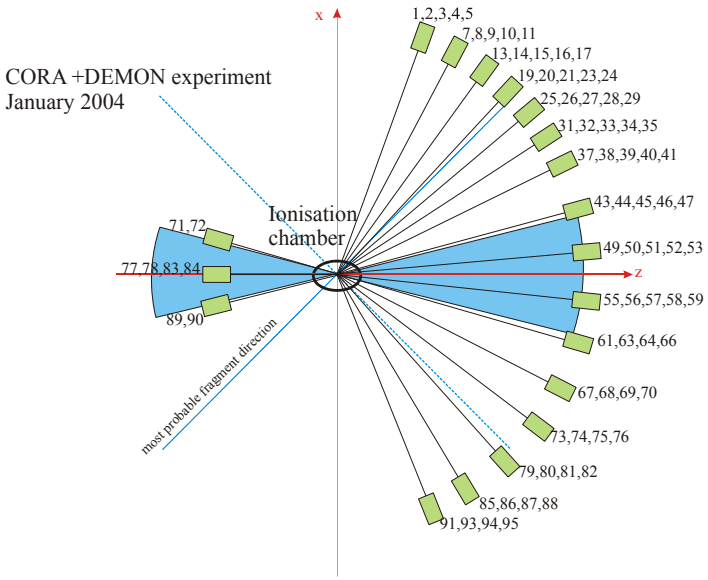

***Рис. 3.** Схема эксперимента по исследованию вылета нейтронов при делении ^{252}Cf.*

Детекторы позволяли отделять нейтроны от гамма-квантов по форме импульса, а также определять энергию нейтрона по времени пролета и угол вылета. В процессе предварительной обработки данных были воспроизведены известные результаты по угловым и энергетическим распределениям нейтронов для ^{252}Cf и, таким образом, отработана и проверена экспериментальная методика. Было накоплено около 10^6 нейтрон-нейтронных корреляций. Исследование таких корреляций совместно с массово-энергетическим и угловым распределениями осколков деления может позволить обнаружить не наблюдавшуюся до сих пор корреляцию вылета нейтрона и направления спина осколков деления, что, в свою очередь, может пролить свет на природу образования спинов осколков в делении. Извлечь такую информацию из тестового эксперимента, по-видимому, не удастся из-за того, что подложка источника деления была повреждена во время его транспортировки. Подобного рода исследования планируются в будущем эксперименте, намеченном на конец 2005 года.

1.2.3 Измерение выходов запаздывающих нейтронов деления

В продолжение работ, направленных на получение данных о выходах и постоянных распада групп запаздывающих нейтронов в делении минорных актинидов, проведена юстировка зеркального нейтроновода на 11Б канале ИБР-2. Разработана методика проведения экспериментов по изучению характеристик запаздывающих нейтронов деления составного ядра ^{246}Cm, позволяющая проводить исследования на ожидаемом уровне фона нейтронов спонтанного деления, собрана ионизационная камера деления с изотопом ^{245}Cm. Проведены комплексные испытания модернизированной установки «Изомер», включающей системы сбора и накопления данных и устройства управления прерывателем нейтронного пучка. Проведены первые измерения на модернизированной установке с ^{235}U и ^{239}Pu.

1.3 Гамма-спектроскопия нейтронно-ядерных взаимодействий

1.3.1 Исследование двухквантовых гамма-каскадов

Решена задача полностью безмодельного определения плотности уровней в фиксированном интервале их спинов и приведенной вероятности возбуждающих и разряжающих их дипольных электрических и магнитных гамма-переходов в диапазоне возбуждений, близком к энергии связи нейтрона. Аналогичных экспериментальных данных в мире не существует.

Реализованная для этого методика использует экспериментальные данные по каскадной заселяемости возбуждаемых при захвате тепловых нейтронов уровней до энергии возбуждения не менее 3-5 МэВ и интенсивности ранее измеренных двухквантовых каскадов на низколежащие уровни тех же ядер. Сопоставление этих данных позволяет экспериментально оценить степень различия энергетических зависимостей радиационных силовых функций первичных и вторичных переходов каскадного гамма-распада компаунд-состояния, и с учетом этого различия, определить без использования каких-либо дополнительных гипотез интервал вероятных значений плотности уровней с минимально возможной в настоящее время ее систематической погрешностью. Такие данные получены для 19 ядер из области $39<A<201$. Основной физический вывод, следующий из их анализа: в большинстве ядер очень существенное изменение структуры возбужденных уровней наблюдается в районах около 20, 50 и 80% энергии связи нейтрона. Эффект проявляется в очень значительном изменении производной от энергетической зависимости плотности уровней и хорошо коррелирующей с ее изменением вариацией радиационных силовых функций одновременно как первичных, так и вторичных гамма-переходов.

В рамках существующих моделей плотности уровней наблюдаемый эффект можно связать только с разрывом двух, как минимум, куперовских пар нуклонов. Но величина эффекта изменения наблюдаемой плотности уровней от энергии возбуждения ядра не

соответствует предсказаниям обобщенной модели сверхтекучего ядра, в первую очередь, по положению точки фазового перехода сверхтекучее-обычное состояния ядра.

1.3.2 Определение схемы уровней изотопов Yb

В 2004 году продолжалось сотрудничество ЛНФ с Пражским политехническим университетом (г. Прага) по анализу результатов, полученных в экспериментах на фильтрованных пучках нейтронов, проводимых на парном спектрометре в Брукхэйвенской национальной лаборатории. Были измерены гамма-спектры радиационного захвата тепловых нейтронов, нейтронов с энергией 2 кэВ и с энергией 24 кэВ. Эти спектры были обработаны и получена обширная информация об уровнях ядра ^{174}Yb. До энергии возбуждения 4 МэВ было обнаружено около 300 уровней. Проводилась подготовка публикации «Levels of Populated ^{174}Yb in Individual Resonance Neutron Capture» по результатам измерений, проведённых в ЛНФ ОИЯИ на реакторе ИБР-30, в которых были получены гамма-спектры из 32 резонансов ^{173}Yb. В работе приводятся значения энергии, спина и четности 77 уровней ядра ^{174}Yb и дается сравнение полученных результатов с имеющимися данными.

1.4 Исследование реакций (n,p) и (n,α)

Проведены методические измерения в рамках подготовки к экспериментам по определению энергетической зависимости коэффициентов углового распределения в реакции ^{14}N(n,p)^{14}C в диапазоне нейтронов ~ 10 кэВ - ~ 1 МэВ. Планируемые исследования интерференционных эффектов s- и p-резонансов в реакции (n,p) представляют интерес как для получения более полной спектроскопической информации о p-резонансах – амплитуды и знаки ширин входного и выходного каналов реакции, зависящие от полного момента частицы j=1/2 и j=3/2, так и для точной интерпретации результатов измерений P-нечетных эффектов. Измерения были выполнены на установке ЭГ-5 ЛНФ ОИЯИ. Нейтроны производились в реакции ^{7}Li(p,n)^{7}Be. Использовалась толстая литиевая мишень и протоны с энергией, на 20 кэВ превышающей пороговое значение. Таким образом, в конусе ~ 120° формировался интегральный нейтронный спектр, по энергетической зависимости близкий к Максвелловскому распределению при средней энергии ~ 30 кэВ. Данные по угловым распределениям для такого спектра важны также для выяснения причин сильного расхождения (в 2-3 раза) значений среднего по Максвелловскому распределению сечения при звездной температуре, полученного в ряде работ. Регистрация и спектрометрия протонов производилась двухсекционной ионизационной камерой с сеткой и электронной системой сбора многомерной информации. В качестве образца применялась адениновая ($C_5H_5N_5$) мишень толщиной 267 мкг/см^2, размером 180 × 160 мм. Получено значение корреляции вперед-назад $\alpha_{fb} = (4.2 \pm 4.0)\cdot 10^{-2}$ без учета вклада фона.

В настоящее время разрабатывается конструкция устройства для поворота и перемещения камеры для проведения основных измерений и оценки фона.

Изготовлены мишени ^{6}Li и Be для совместных экспериментов по исследованию реакции (n,α) в Пекинском университете. Для продолжения исследований реакций (n,p), (n,α) на быстрых нейтронах на ЭГ-5 конструируется газовая дейтериевая мишень.

Начаты работы по подготовке к исследованию «нестатистических» эффектов в α-распаде нейтронных резонансов ^{147}Sm на спектрометре по времени замедления в свинце СВЗ-100 ИЯИ РАН в Троицке.

1.5 Программа ядерных данных

1.5.1 Исследование резонансной структуры нейтронных сечений

В 2004 г продолжалась обработка времяпролетных спектров, ранее измеренных на 122 м, 501 м и 1006 м пролетных базах ИБР-30 с помощью многосекционных детекторов нейтронов и гамма-лучей для Nb, Mo, Pb, ^{235}U (77 К и 293 К) образцов-фильтров. Из времяпролетных спектров после вычитания фона определялись полные и парциальные нейтронные групповые сечения и факторы резонансной блокировки полного сечения и сечения рассеяния в диапазоне энергий 100 эВ - 200 кэВ для Nb, Mo, Pb. Экспериментальные погрешности сечений и факторов блокировки составляют, соответственно, 3-7% и 8-15%. Аналогичные величины были определены расчетным путем по программе ГРУКОН на основе оцененных данных разных библиотек. В целом расчетные и экспериментальные данные совпадают, но в некоторых энергетических группах расхождения выходят за пределы экспериментальных ошибок.

Для урана-235 из времяпролетных спектров разной кратности совпадений гамма-лучей после вычитания фоновых составляющих определялся допплер-эффект в величине альфа при температурах 293 К и 77 К. Экспериментальные погрешности в величине альфа составляют 2-10% в зависимости от резонансных особенностей величины альфа. Проведены расчеты альфа величины на основе оцененных данных разных библиотек по программе ГРУКОН. Различия расчетных и экспериментальных величин достигают 30% в некоторых резонансах и энергетических группах. Конечные результаты этих исследований представлялись на научных международных семинарах и конференциях в России, Румынии, Польше и Турции. Эти работы выполнены в рамках сотрудничества ЛНФ (Дубна), ФЭИ (Обнинск), ИЯФИЯЭ (Болгария), Лодзинский университет (Польша).

Продолжена работа по созданию установки на ИБР-2 по монохроматизации тепловых и холодных нейтронов и укорочению вспышки быстрых нейтронов с помощью механических прерывателей нейтронов. Проведены измерения полных сечений на пучке 6Б ИБР-2 в области холодных нейтронов.

1.5.2 Ядерные данные для ADS и изучение тонкой структуры вибрационных резонансов на пороге деления

В течение последних трех лет на n_TOF нейтронном источнике ЦЕРНа в рамках широкой международной коллаборации совместно с коллегами из ФЭИ, Обнинск, были исследованы сечения деления для высоко обогащенных изотопных мишеней ряда актинидов в широкой области энергий нейтронов. Программа исследований была направлена на получение новых (или уточнение существующих) данных для управляемых ускорителями подкритических систем (ADSS), а также на изучение фундаментальных аспектов ядерного деления.

В 2004 году измерения были проведены для образцов ^{241}Am, ^{243}Am и ^{245}Cm с помощью быстрой ионизационной камеры FIC1, используя для калибровки мишени ^{235,238}U. Кроме того, с помощью модернизированной ионизационной камеры FIC0, дополненной сеткой, позволяющей наряду с сечением деления измерять также разницу в выходах осколков деления по и против направления нейтронного пучка (так называемую вперед-назад угловую корреляцию), были проведены измерения с образцом ^{236}U. Данные, полученные в октябре-ноябре 2004 года, анализировались вместе с результатами измерений 2002-2003 г.г. для образцов ^{234,236}U, ^{232}Th, ^{237}Np. Ниже приводятся некоторые предварительные результаты этого анализа для интервала энергий нейтронов 1 эВ- 1 МэВ.

Сечение деления для ядра-мишени ^{234}U, измеренное на источнике n_TOF ЦЕРН, оказалось в удовлетворительном согласии с ENDFB данными до энергий ниже 1,5 кэВ. Для более высоких энергий, благодаря отличному энергетическому разрешению источника, было обнаружено много новых уровней второй ямы. Кроме того, были получены надежные

доказательства существования тонкой структуры вибрационных резонансов на пороге деления (см. **рис. 4а**).

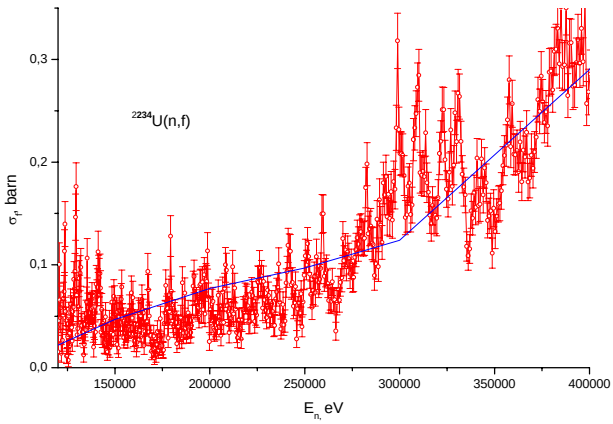

Рис. 4а

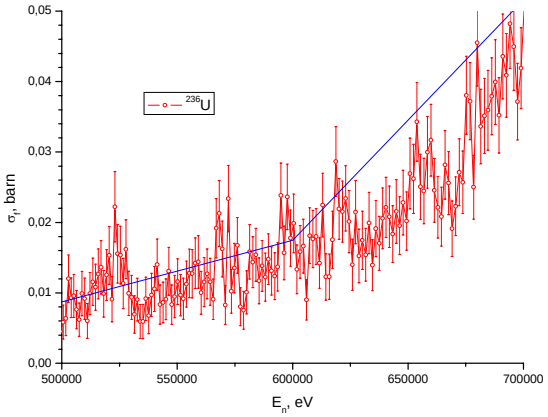

Рис. 4б

Весьма интересные результаты были получены для ядра-мишени ^{236}U. Обнаружены существенные расхождения с оцененными данными ENDFB. В частности, в интервале энергий от 5 эВ до 1, 2 кэВ не было наблюдено ни одного нейтронного резонанса, тогда как в ENDFB файле их приводится несколько десятков. Кроме того, для одного из компаунд-уровней триплета, расположенного около 1,2 кэВ, обнаружено сильное увеличение проницаемости барьера деления, связанное, по-видимому, с квантовыми резонансными эффектами. Как и для ядра-мишени ^{234}U, в случае ядра ^{236}U надежно установлено существование тонкой структуры околобарьерных вибрационных состояний, иллюстрируемое **рис. 4б**.

Для ядра-мишени ^{237}Np полученные сечения деления не находятся в достаточном согласии с оцененными данными ENDFB. В области энергий нейтронов около 40 эВ разница сечений достигает шести раз. Это приводит к изменению резонансного интеграла сечения деления, величина которого является важной для систем трансмутации радиоактивных отходов. Кроме того, в энергетическом интервале 500-700 кэВ получена примерно 7%-я разница между ENDFB данными и n_TOF сечениями. Это различие вполне значимо для оценки баланса нептуния в быстрых реакторах. Выше 500 эВ впервые наблюдено много новых уровней второй ямы для компаунд-ядра ^{238}Np. Эти данные позволят уточнить характеристики барьеров деления для данного ядра и лучше понять связь компаунд-уровней первой и второй деформационных ям.

1.6 Фундаментальные свойства нейтрона

1.6.1 Исследования дифракции нейтронов в газах

Важным способом изучения межатомных взаимодействий является наблюдение дифракции нейтронов в газах и жидкостях и получение их структурных факторов $S(q)$ ($\hbar q$ - переданный импульс). При получении $S(q)$ из экспериментальных данных по рассеянию вводятся разнообразные поправки, в том числе, на вклад в рассеяние n,e-взаимодействия считающегося известным. В публикациях предыдущего года (ОИЯИ, Е3-2003-183 и Р3-2003-232) был продемонстрирован новый метод определения b_{ne}, основанный на том, что интенсивность дифракции $S(q)$ в первом приближении пропорциональна плотности атомов газа n (его давлению), а относительный вклад n,e-рассеяния от плотности газа не зависит. “Обратным ходом”, используя литературные данные по $S(q)$ криптона при разных n и информацию о поправках, были получены исходные интенсивности рассеяния, обработка

которых и позволила надежно выделить эффект n,e-рассеяния. Однако, из-за неопределенности нормировочной константы в описании абсолютных интенсивностей рассеяния надежного значения величины b_{ne} получено не было.

В 2004 году был найден способ обойти трудность, связанную с неполной информацией о поправках. Удалось получить математическое описание непосредственно данных по $S(q)$, в которое величина b_{ne} входит свободным параметром. При этом использовались все данные до самых больших n, а в описание был включен член с n^2. Дифракция описывалась подобранными функциями, которые обеспечивали нужные осцилляции $S(q)$, затухающие с ростом q и содержащие по 4 свободных параметра в членах с n и n^2. Десятым свободным параметром была вышеупомянутая нормировочная константа.

Одновременная подгонка 10 параметров по 1326 значениям $S(q)$ (78 разных q при 17 разных n) позволила получить такой результат: $b_{ne} = -(1.53 \pm 0.24) \cdot 10^{-3}$ Фм. Его следует рассматривать как новый, хотя и довольно скромный по точности. При этом его надежность (т.е. отсутствие больших систематических ошибок) определяется надежностью использованных данных по $S(q)$.

1.6.2 Измерение длины n,e-рассеяния

В практическую фазу перешло сооружение новой установки для измерения b_{ne} классическим методом, предложенным еще Ферми, но с применением метода времени пролета, что многократно повышает надежность результатов. В установке будут работать четыре нейтронных детектора, которые уже изготовлены и налажены. Каждый из них – пропорциональный ^{3}He-счетчик с давлением ~8 атм, снабженный предусилителем и помещенный в защиту из борированного полиэтилена и кадмия. С одним из детекторов были проведены тестовые измерения в Троицке на вертикальном нейтронном пучке, получаемом от пробной мишени.

Разработаны рабочие чертежи юстировочно-поворотного устройства, с помощью которого будет достигаться совмещение оси камеры рассеяния с осью пучка (вертикального и горизонтального), а затем в процессе измерений камера рассеяния с детекторами будет периодически поворачиваться на 180^0, так что каждый детектор будет попеременно регистрировать рассеяние вперед и назад.

Успешный опыт описания дифракционной части рассеяния математическими формулами и желание иметь дело с как можно большим перепадом электронного форм-фактора способствовали тому, что был разработан проект нового эксперимента. Для его реализации достаточно одной невысокой плотности газа (с давлением 1-3 атм), но энергия монохроматического пучка нейтронов должна быть в пределах ~ 50 – 200 мэВ (λ~ 1.3 – 0.6 ангстрем). Тогда для задних углов рассеяния можно будет достигать передаваемых волновых чисел ~ 10–20 обратных ангстрем и, соответственно, довольно малых значений форм-фактора (0.36–0.19 для криптона).

Одновременно, для устранения влияния разброса эффективностей детекторов в качестве стандартного рассеивателя предлагается использовать не ванадий, а инертный газ неон с меньшим вкладом n,e-рассеяния, который дает эффект от теплового движения атомов той же природы, что и основной газ.

1.6.3 Эксперимент по прямому измерению длины рассеяния нейтрона на нейтроне на импульсном реакторе ЯГУАР (Снежинск)

Для проверки правильности расчетов и выбора оптимального варианта защиты под реактором было выполнено тестовое измерение. Для проведения измерения были изготовлены:

- штатный замедлитель, штатный головной коллиматор и компоненты защиты под реактором, выполненные из борированного полиэтилена и трубчатых коллиматоров;
- система регистрации, состоящая из детекторов тепловых и быстрых нейтронов – газовых пропорциональных счётчиков с ^{3}He и ^{4}He с предусилителями;
- разработана и изготовлена система позиционирования нейтронных детекторов внутри канала с дистанционным управлением.

На **рис. 5** представлена схема этого измерения. Замедлитель, толстый конический коллиматор и защита под реактором здесь точно такие, как и в полной схеме эксперимента, но отсутствует вакуумный канал и коллимационная система. Детекторы в подреакторной шахте могут устанавливаться в любой точке шахты.

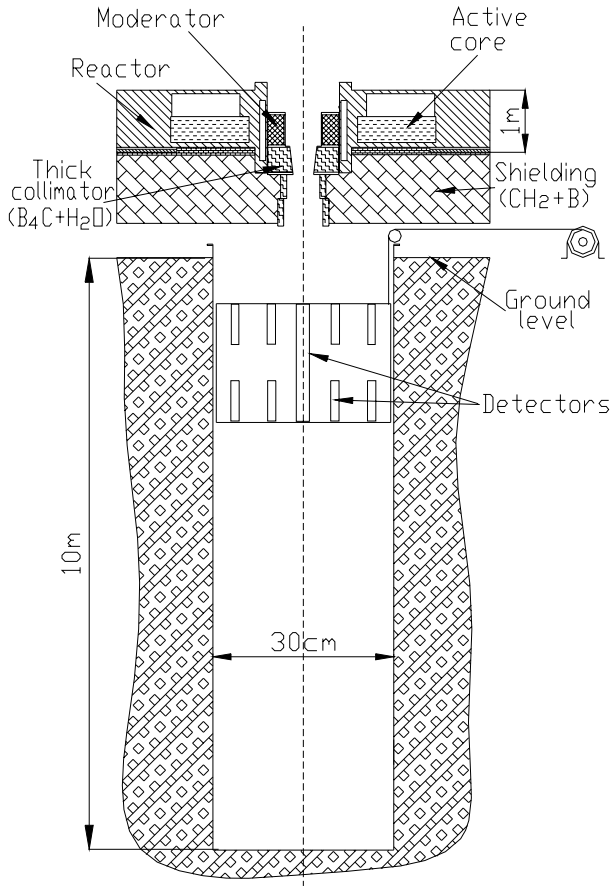

***Рис. 5**. Схема тестового измерения.*

Измерения проводились в стационарном режиме работы реактора. Были измерены плотности потока для трех групп нейтронов: тепловых – с энергией ниже кадмиевого резонанса, эпитепловых – с энергией выше кадмиевого резонанса, и быстрых, с энергией ~ 1 МэВ. Измерения проводились по всей глубине шахты, для трех различных геометрий и типов коллиматоров, чтобы иметь больше информации для сравнения расчетов с экспериментом. На **рис. 6** представлены предварительные результаты для зависимости плотности потока тепловых нейтронов от глубины шахты для двух разных геометрий коллиматора. Как видно, результаты расчетов хорошо согласуются с измерениями.

Измерение плотности потока нейтронов низких энергий представляет интерес для сравнения с расчетами. В этом случае счет детектора в основном определяется рассеянием на воздухе в канале, и он на много порядков выше ожидаемого для случая вакуумного канала. Для тестирования защиты под реактором наибольший интерес представляют измерения

плотности потока быстрых нейтронов. Эти измерения выполнены, но окончательно не проанализированы, так как пока нет калибровочных измерений эффективности использованного детектора быстрых нейтронов. В ближайшее время планируется их провести.

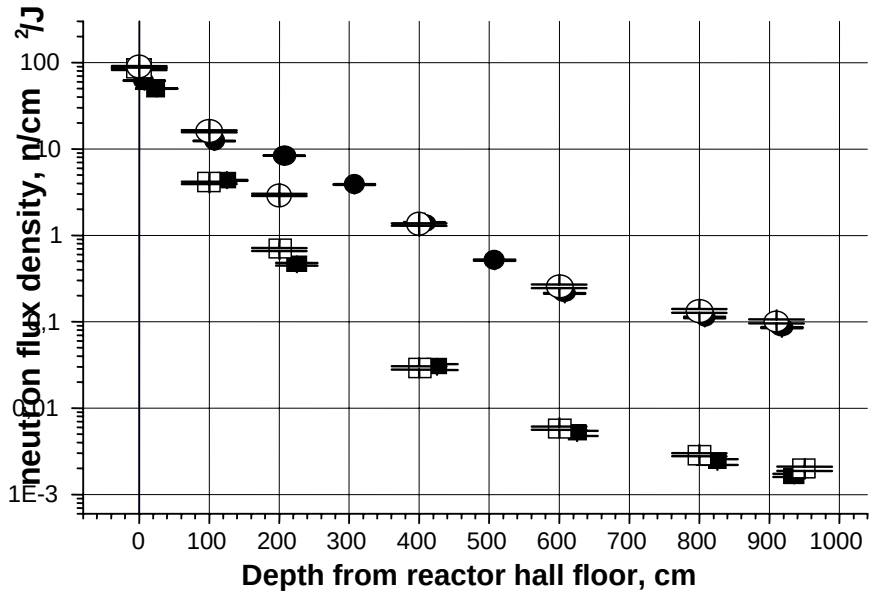

Рис. 6. *Плотности потока тепловых нейтронов на 1 Дж в подреакторной шахте в зависимость от ее глубины. Темные точки – результаты измерений, пустые точки – расчеты. Кружки и квадраты соответствуют разным геометриям коллиматора.*

Изготовлена «задняя» (противоположная от детектора) пролётная база нейтронного канала экспериментальной установки. Были проведены вакуумные испытания данной части канала, затем вся внутренняя поверхность покрыта кадмием толщиной 1 мм и проведены повторные вакуумные испытания. Задняя пролётная база перевезена в г. Снежинск.

В 2005 году планируется изготовить и смонтировать на реакторе всю экспериментальную установку и проверить её работоспособность.

1.6.4 Поиск новых взаимодействий нейтронов с ядрами

Из анализа экспериментов по рассеянию нейтронов получены ограничения на константу взаимодействия типа Юкавы как гипотетической поправки к Ньютоновскому гравитационному потенциалу. Ограничения получены для радиуса взаимодействия между 10^{-12} и 10^{-7} см, где эксперименты по измерению сил Казимира и с применением атомной силовой микроскопии не чувствительны. Получены также экспериментальные ограничения на величину неэлектромагнитных степенных нейтрон-ядерных потенциалов. Обсуждены некоторые возможности усиления ограничений.

1.7 Физика ультрахолодных нейтронов, нейтронная оптика

1.7.1 Дифракция на движущейся решетке как нестационарное квантовое явление

На источнике УХН в Институте Лауэ-Ланжевена (Гренобль, Франция) поставлен новый эксперимент по измерению спектров УХН, возникающих в результате дифракции на движущейся решетке. В отличие от первого демонстрационного опыта, новый эксперимент позволяет провести количественное сравнение с теорией. Как и ранее, первичная монохроматизация пучка и анализ возникающих спектров осуществлялся с помощью интерферометров Фабри-Перо, а используемым прибором был гравитационный спектрометр с ФП интерферометрами. В эксперименте уверенно наблюдался эффект квантования энергии, возникающий как следствие фазовой модуляции нейтронной волны, поперек которой движется фазовая решетка. Измеренная величина расщепления спектра, определяемая частотой модуляции, совпадает с расчетом с двухпроцентной точностью, а дифракционная эффективность решетки (интенсивность волн первого порядка) составила 38%, что близко к предельно возможной величине для этого типа решеток. Неизменность ширины спектральной линии при приведении решетки во вращение позволяет оценить снизу поперечные размеры плоского волнового фронта исходной волны. Такая поперечная длина когерентности составляет величину, не меньшую, чем 0.07 см, что в тысячу раз превышает длину волны нейтрона (**рис. 7**).

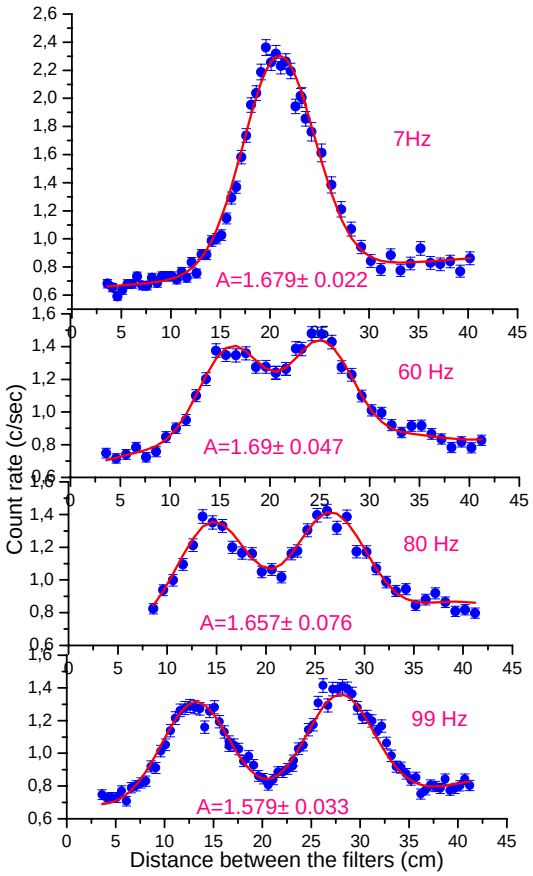

***Рис.** 7. Трансформация спектра УХН при пропускании через вращающуюся решетку. Частота вращения указана на графиках.*

Вращающаяся решетка с пространственным периодом α зависящим от ее азимутального угла, была использована для активного воздействия на энергию и скорость нейтрона для осуществления фокусировки нейтронов во времени. При этом в течение первой половины оборота решетки условию фокусировки удовлетворяют нейтроны с энергией $\mathbf{E(t) = \hbar[\omega - \Omega(t)]}$, где $\mathbf{\Omega = 2\pi f\alpha^{-1}}$ - частота модуляции, f – частота вращения решетки. Во время второй половины оборота решетки условию фокусировки удовлетворяют нейтроны с энергией $\mathbf{E(t) = \hbar[\omega + \Omega(t)]}$. В результате нейтроны, поступающие в установку в случайные

моменты, достигают точки детектирования, группируясь вокруг определенного момента времени – точки временного фокуса. Полученная к настоящему времени эффективность такой фокусировки составляет примерно 28% (**рис. 8**).

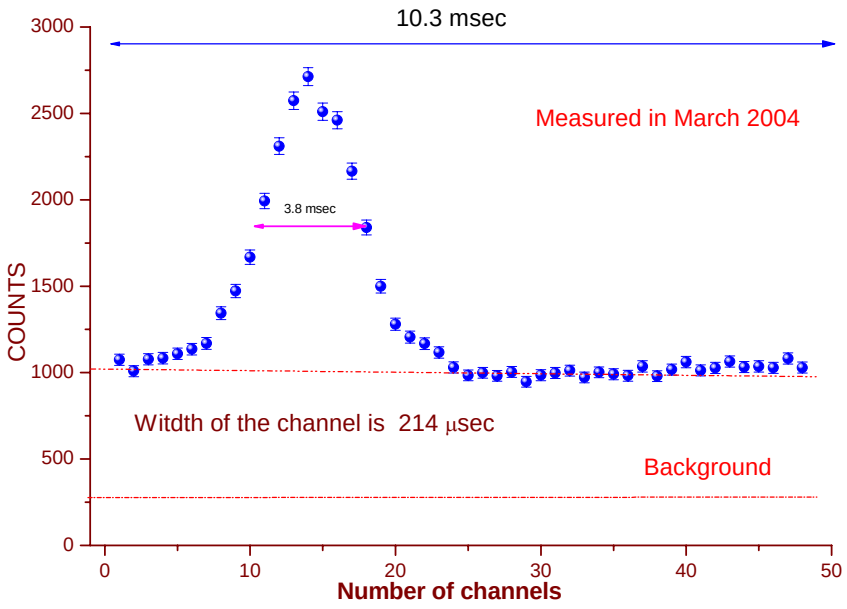

***Рис. 8**. Пик временной фокусировки.*

1.7.2. Квантовые эффекты в одномерной гравимагнитной ловушке

Решена задача о хранении ультрахолодных нейтронов над плоским магнитным зеркалом Владимирского в присутствии гравитации. Для нейтронов с определенной поляризацией суммарный магнитный и гравитационный потенциал может иметь минимум, образуя гравимагнитную ловушку. При малых энергиях вертикального движения состояние нейтрона в такой яме оказывается квантованным. При вполне реалистических значениях параметров магнитного зеркала волновые функции первых нескольких состояний оказываются локализованными в области размером несколько десятков микрон. Положение области локализации чувствительно к величине ускорения свободного падения нейтрона.

1.7.3. Исследования времени жизни нейтрона и аномальных потерь при хранении УХН

За прошедший год были заново изготовлены ловушка УХН из монокристаллического сапфира длиной 30 см и диаметром 3.6 см и новая установка, позволяющая измерять время хранения УХН в ловушке в диапазоне температур (80 – 800 К). Были проведены измерения на источнике УХН в ИЛЛ (Франция). Программа измерений была полностью выполнена. Наилучшее значение фактора потерь УХН, полученного в этой ловушке, на порядок больше предсказываемого теорией. Чтобы понять причину этого расхождения, необходимо провести дополнительные исследования.

Проведен этап измерений (совместно с ПИЯФ и ИЛЛ) времени жизни нейтрона с точностью, лучше 1 с: $878.5 \pm 0.7 \pm 0.3$ сек. Этот результат отличается от среднего мирового значения на 6 стандартных отклонений. Однако новое значение для времени жизни нейтрона совместно с асимметрией вылета электронов, находится в хорошем согласии со Стандартной моделью.

1.7.4. Исследования по разработке источников ультрахолодных нейтронов

Проведен эксперимент (совместно с Институтом Пауля Шерера и ИЛЛ) по прямому измерению генерации УХН в газообразном, жидком и твердом дейтерии в диапазоне температур 10 - 80 К. Полученный результат согласуется с расчетами в некогерентном приближении. Проведены детальные расчеты генерации УХН и энерговыделения в замедлителях на импульсном реакторе «TRIGA», проведены многочисленные измерения тепловыделения в различных материалах и сравнение с расчетами. Предложен простой метод и проведены расчеты транспорта очень медленных нейтронов в холодном замедлителе с быстро меняющейся температурой. Рассмотрен также транспорт нейтронов в гранулированной среде. Расчеты применимы для оптимизации замедлителей ультрахолодных и очень холодных нейтронов на импульсных источниках.

2. Теоретические исследования

2.1. Теоретические исследования β-распада нейтрона

Уровень исследований в физике электрослабых взаимодействий в настоящее время требует надежного знания характеристик β-распада нейтрона с точностью ~ 0.1%. В соответствии с этим, в 2004 году продолжались исследования, имеющие целью достичь наилучшей точности в определении радиационных поправок к распаду нейтрона.

Для корректного вычисления радиационных поправок в расчеты включено калибровочно-инвариантное взаимодействие нуклонов с электромагнитным полем на основе модели векторной доминантности. Структура нуклона эффективно учитывается в этом подходе тем, что наряду с непосредственным взаимодействием электромагнитного поля с изовекторным и изоскалярным нуклонным током, включается также калибровочно-инвариантное взаимодействие электромагнитного поля с нуклонами через посредство векторных ρ, ϕ, ω-мезонов. Такой учет структуры нуклона в рамках модели векторной доминантности приводит к форм-факторам вида $-m_\rho^2/(k^2 - m_\rho^2)$ во всех электромагнитных вершинах, а также к дополнительным вкладам в радиационные поправки, обеспечивающим калибровочную инвариантность расчета поправок.

Структура нуклона учитывается в наших исследованиях радиационных поправок также методами алгебры токов. При вычислении радиационных поправок оказывается возможным в общем виде, с учетом сильных взаимодействий, связать функцию распространения нуклона с электрослабыми нуклонными вершинами.

Выполненная работа позволяет надежно судить о величине радиационных поправок с точностью ~ 0.1%, что необходимо для дальнейшего уточнения характеристик электрослабых взаимодействий, извлекаемых из обработки экспериментальных данных.

2.2 Теоретические исследования парных корреляций нейтронов деления

Проведено теоретическое исследование парных корреляций нейтронов с малыми относительными импульсами ($0 \le |\mathbf{q}| \le 100$ MeV/c), образующихся в процессе деления тяжелых атомных ядер ($A \ge 200$). При этом использован общий метод парных импульсных корреляций частиц с малыми относительными импульсами в рамках модели точечных одночастичных источников. Парные корреляции нейтронов обусловлены в общем случае как эффектом Ферми-статистики, так и *S*-волновым сильным взаимодействием в конечном состоянии (последнее имеет место только для синглетного состояния нейтронной пары). Установлено, что для обычных нейтронов деления (испущенных из фрагментов), парные корреляции при ненулевых относительных импульсах практически отсутствуют, ввиду большой разности

времен эмиссии (> 10^{-19} сек), и двухнейтронная корреляционная функция чувствительна к эффектам Ферми-статистики и взаимодействия в конечном состоянии только для пар мгновенных (“pre-scission” и “scission”) нейтронов (соответствующие времена эмиссии – порядка $10^{-21} \div 10^{-22}$ сек, размеры области эмиссии – порядка нескольких Фм). Таким образом, корреляционный метод в принципе может быть применен для определения доли пар мгновенных (“pre-scission” и “scission”) нейтронов в общем количестве нейтронных пар, фиксируемом при делении.

3. Аналитические исследования на реакторе ИБР-2

3.1 Экология, биотехнологии, материаловедение

В 2004 году были продолжены работы по изучению атмосферных выпадений тяжелых металлов с применением техники биомониторирования, НАА и ГИС технологий (проект РЕГАТА) на территории Центральной России (Тульская, Тверская, Ярославская и юго-восток Московской областей), а также Армении (Севан) и Вьетнама. Проведены организационные и методические работы по подготовке к очередному европейскому одновременному сбору мхов-биомониторов (moss-survey) атмосферных выпадений тяжелых металлов в 2005 году в ряде стран-участниц и неучастниц ОИЯИ (Белоруссия, Украина, Болгария, Босния, Македония, Польша, Румыния, Сербия, Словакия, Турция (европейская часть).

Проведен сравнительный анализ различных биомониторов (лишайников, коры деревьев) и почвы из района нефтеперерабатывающего завода в Констанце, Румыния. Показана возможность использования биомониторов для оценки воздействия этого предприятия на окружающую среду курортной зоны Черноморского побережья Румынии.

Проведен НАА более чем 250 образцов растительного и животного происхождения в рамках координационной программы (2002-2005) и проекта Технической кооперации с МАГАТЭ (2003-2005) по контролю и качеству продуктов питания, выращенных в условиях сильного антропогенного загрязнения.

В 2004 году выполнен заключительный этап работ по проекту «Мониторинг на рабочих местах и здоровье персонала, занятого в производстве фосфорных удобрений на ряде заводов России, Узбекистана, Польши и Румынии» (Европейская Программа 5, Коперникус). Результаты анализа экологических образцов (сырья, почвы, донных отложений, воды и воздушных фильтров) и биосубстратов человека (волосы, ногти, моча и зубы) докладывались на двух международных конференциях и направлены в печать.

Продолжены совместные работы с группой биофизиков Института физики АН Грузии по разработке новых медицинских препаратов и сорбентов на основе сине-зеленой водоросли *Spirulina platensis.* Часть этих исследований была проведена на реакторе Университета в Техасе, США. В 2004 году получен патент на способ получения биомассы спирулины, содержащей хром.

Проведен анализ 70 археологических образцов керамики и стекол из музея в Констанце, Румыния, с целью их идентификации.

Завершен анализ данных по изучению влияния нейтронов спектра деления на физические свойства мелкокристаллических алмазов, полученных в Институте физики твердого тела и полупроводников НАН Белоруссии (Минск).

2. NEUTRON SOURCES

2.1. THE IBR-2 PULSED REACTOR

In the year 2004 the IBR-2 reactor operated ~1384 hours for physical experiments (see Table 1).

Table 1

The operation parameters of the IBR-2 reactor in 2004

Cycle №	**1**	**2**	**3**	**4**	**TOTAL:**
Time of cycle	13.09 - 24.09	18.10 - 05.11	15.11 - 26.11	06.12 - 24.12	
1. Operation for physical experiment, hr	264	418	268	434	**1384**
2. Operation of MR-3, hr	273	434	275	443	**1425**
3. Generated power, MWt·hr	402	633	404	653	**2092**
4. Number of emergency shutdowns (AES)	1	2	–	–	**3**
5. Due to:					
5.1. Voltage drops	–	2	–	–	**2**
5.2. Instrumental malfunction or failure	1	–	–	–	**1**
5.3. Electronic equipment failure	–	–	–	–	**–**
5.4. Personnel error	–	–	–	–	**–**

Main results of the IBR-2 modernization in 2004:

1) MR-3 – chief task of the year.

At the beginning of February, 2004, the MR-3 assembling was fully completed on the FLNP test-bench and MR-3 was started up at rated speed (**Fig.1**). The MR-3 investigation program to measure vibration characteristics in the modes of 5 and 10 Hz was carried out. All MR-3 parameters corresponded to the engineering requirements. A life test was also carried out and it revealed no deviations in the MR-3 operation, all systems functioned correctly. Later the machine was moved into the reactor building.

The MR-3 assembling was carried out at the regular place near the reactor, tests were conducted, MR-3 was approved to be put into service by Gosatomnadzor.

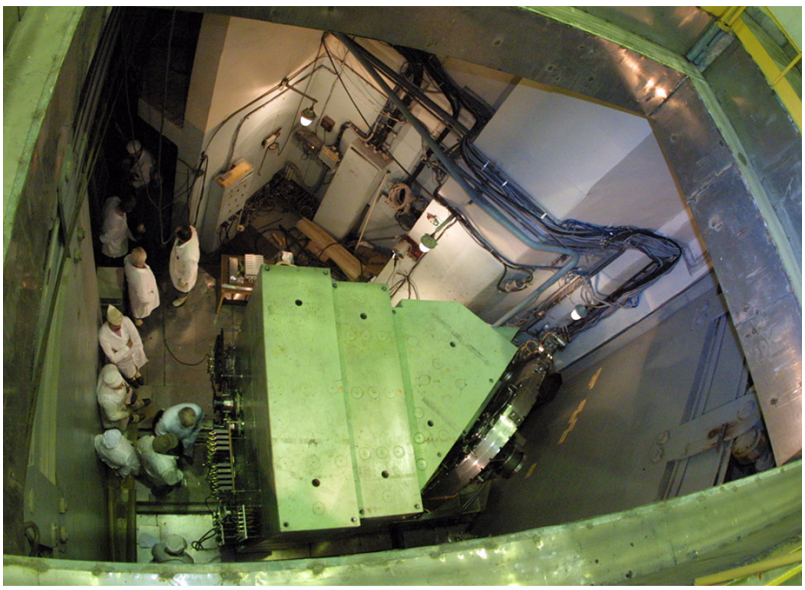

Fig.1. *MR-3 before assembling at the regular place.*

From 16.06.2004 to 23.07.2004 the Program to start and investigate the main characteristics of the IBR-2 with a new MR-3 was performed: the efficiency curve of the movable reflector was measured in the stationary mode, (see **Fig. 2**) efficiencies of the adjustment units were measured, the efficient reactivity margin was determined, an additional load of the reactor by one fuel assembly was carried out, pulse shape and pulse fluctuations up to 1.5 MWt were measured. The obtained results are close to the calculated ones. (see **Figs. 3,4**).

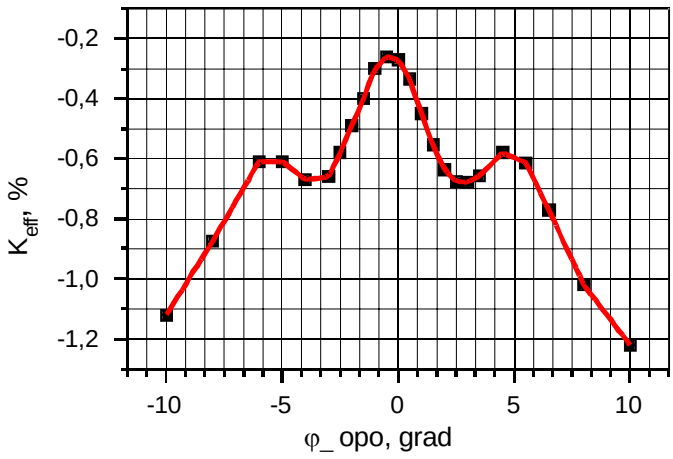

Fig. 2. *Reactivity variation at the MR-3 rotor displacement in the range ± 10 degrees of the main moveable reflector. X-coordinate represents the main moveable reflector displacement in degrees, Y-coordinate – deviation of the multiplication coefficient from unit.*

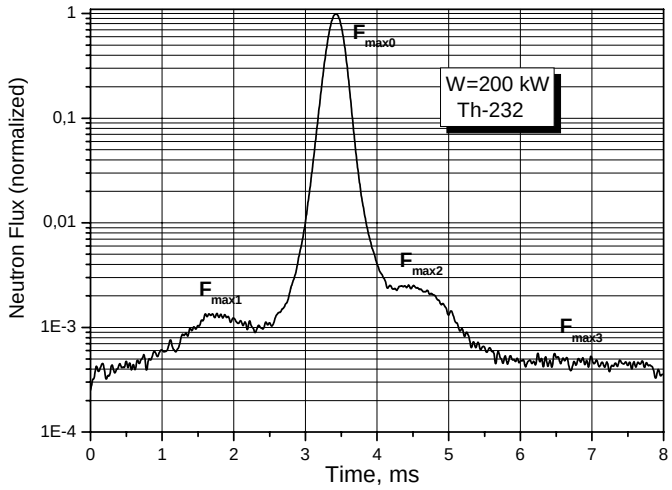

Fig.3. *Pulse shape of power. The data are normalized for the pulse maximum. Measurements are performed with the help of Th-232 - chamber.*

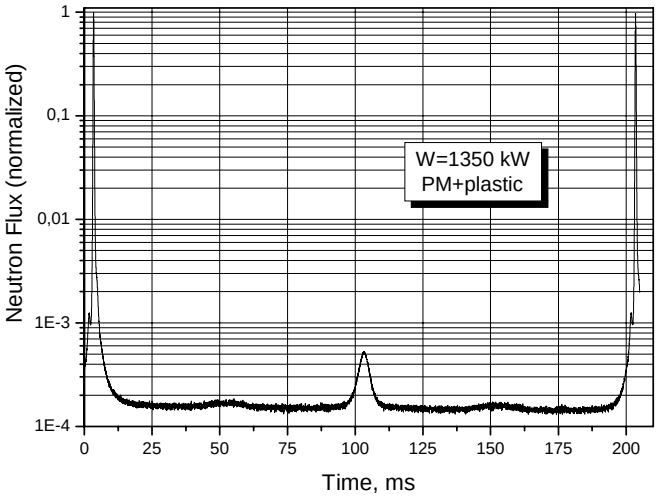

Fig.4*. Power distribution between two successive flashes. The data are normalized for the flash maximum. Measurement is performed with the help of scintillation detector.*

Thus, a very important stage of the IBR-2 modernization to create a new MR-3 was completed.

On 13.09.2004 an operation for physical experiment in accordance with the working schedule started.

2) Manufacturing of fuel elements was completed at the industrial enterprise «Mayak». In April, 2004, the fuel elements were delivered to JINR. The works to prepare a working floor for the assembling of the fuel elements into a fuel assembly are under way.

3) Works on the development of design documentation for stationary reflectors and rolling shieldings were completed.

4) Manufacturing of a new reactor jacket continued in NIKIET. Manufacturing of rolling shieldings and stationary reflectors started in JINR EW.

5) Development of design documentation (DD) on CSS of the IBR-2 continued.

To provide for the works on the IBR-2 modernization in 2004, a sum of 696 k$, including JINR – 348 k$, Federal Agency on Atomic Energy – 348 k$, was spent.

«Development of complex of the neutron moderators of broad spectrum («combi-moderators») for the modernized research reactor IBR-2M»

1. The facility has been manufactured and the experiments to measure hydrogen pressure in the moderator chamber with mesitylene at irradiation in the conditions imitating the operating ones (on the microtron MT-25 FLNR) have been conducted. The analysis has showed that in the designed mesitylene-based moderator the maximal pressure on the shell on heating of mesitylene may amount to 25 bar after a day of operation. This result gives the initial data for choosing the parameters of the moderator fuel elements. The paper is submitted for publication in JINR Communications.
2. Development of the optimal configuration of moderators at the directions of 4, 5, 6, 1 and 9-th beams (**Fig.5**), and of the 2-nd and 3-rd beams, has been completed. By way of calculation the values of spectral density of neutron fluxes (**Fig. 6**), which are much higher in the region of short waves, and in the region of cold neutrons – are at the level of the designed solid methane moderator of the second target of the ISIS source. Thus, along with the earlier made optimization of combi-moderators for the 7-th, 8-th, 10-th и 11-th beams, composition of the whole moderator complex has been developed. Preparation of the report for the international conference ICANS XVII, USA, April 2005, is under way.
3. The principle of tube design of mesitylene cold moderator has been developed, providing, at the least, no less than 3-4 days of continuous operation without hydrogen annealing and general long-term operating life of the IBR-2M. E.P. Shabalin, S.A. Kulikov, JINR Communications, P13-2004-73.
4. Requirements specification to design the moderator complex along with NIKIET has been worked out.
5. Laboratory experiments to search for the technique to prepare balls of solid mesitylene of 10-15 mm in diameter have been started. In the case of positive result the moderator design may be simpler, cheaper for manufacturing and more convenient in service.

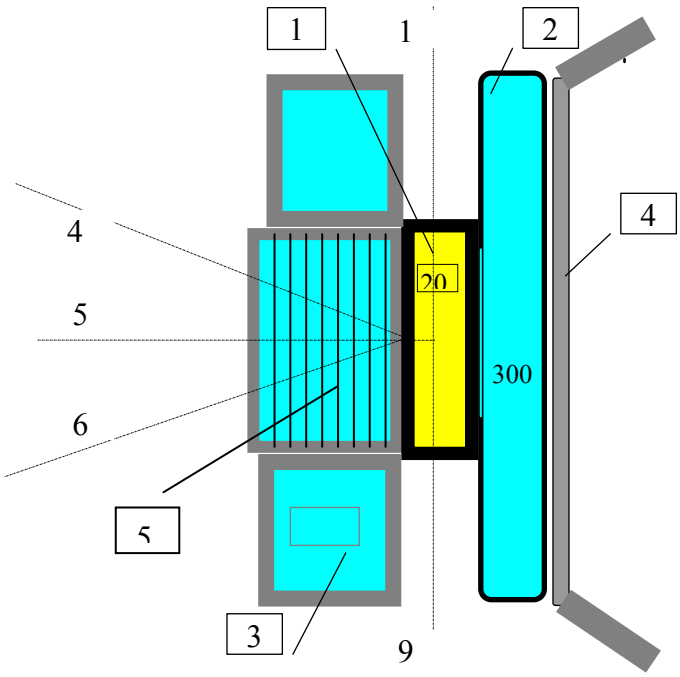

Fig.5. *1 – cold moderator; 2 – pre-moderator; 3 – flat post-moderator; 4 – boundary of the reactor; 5 –comb post-moderator.*

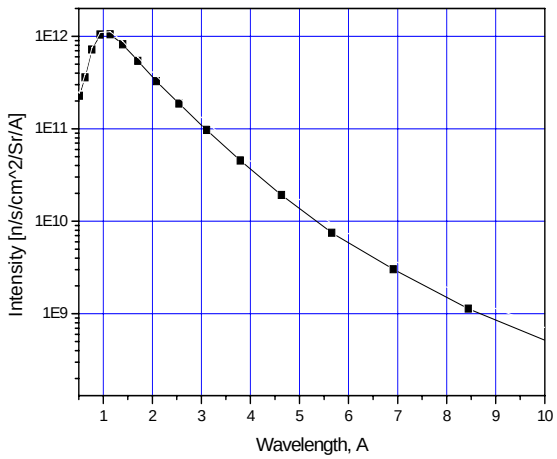

Fig.6. *Differential neutron flux density from the ends of cold moderator (beams 1 and 9).*

Plans for 2005

1. Assembling of fuel elements into fuel assemblies.
2. Continuation of works to manufacture the new reactor jacket and other main equipment.
3. Development of the CSS electronic equipment of the IBR-2M and of the CSS actuating mechanisms.
4. Development of the engineering design of the moderator complex for the IBR-2M.
5. Manufacturing of CHF.

2.2. THE IREN PROJECT

The IREN project working plan for 2004 included:

1. completion of IBR-30 dismantling
2. shipment of fuel for the multiplying target from the industrial enterprise “Mayak” to JINR;
3. assembling of the main equipment of the linac LUE-200 in bldg. 43.

The amount of minimal financing to implement the plan is 250k$. In fact, in March about half requested amount with guaranteed financing of the first two stages only was assigned. In addition, a considerable sum (about 50 k$) was to be paid to NIKIET for the preparation of design documentation for manufacturing of the IREN multiplying target performed in 2002-2003.

Up to mid-August the implementation of the working schedule for dismantling of the IBR-30 reactor was carried out with insignificant delays in spite of a very difficult financial situation in JINR. However, on 19.08.04 the decision of the Government of the Russian Federation on the reorganization of some Russian authorities (including Gosatomnadzor and the Ministry of Ecology) responsible for licensing of activities in the field of atomic energy use was enforced. The decision delayed considerably the granting of a license for putting into operation of the storage area for IBR-30 radioactive elements in bldg. 117/6 making it impossible to complete the IBR-30 dismantling in 2004.

The negotiations with the representatives of the reorganized Rostekhnadzor, which includes the former Gosatomnadzor, show that the necessary licenses may be granted in the first quarter of 2005 and, correspondingly, the dismantling of the reactor may be performed starting from next summer. It is important to note that the works outlined in the 2004 working plan as to be implemented by the FLNP services have been successfully completed.

A large amount of work to prepare the transportation of fuel for the IREN multiplying target has been carried out. On December 8, 2004, the fuel was delivered from the industrial enterprise "Maiak" to JINR.

Due to practical absence of financing, works to mount the equipment for the linac LUE-200 were mainly implemented with the help of internal resources. However, certain advances were made in the construction of the electron gun, focusing elements and RF systems. The pulsed electron source was finally adjusted to the designed parameters, which was proved by its successful testing. The main equipment of the RF modulator was installed at a regular place in the accelerator halls of bldg. 43, FLNP. At the full-scale RF test-bench the system of doubling the klystron power supply was successfully tested. But the absence of funds for purchasing the necessary cables and a number of components led to a delay in the completion of mounting of the main equipment of the linac LUE-200.

The manufacturing of the elements for the magnetic focusing system in LPP and VBLHE stopped in September due to lack of financing. By now about 70% of the whole focusing system has been manufactured. Testing of its elements at the recently created LPP stand for magnetometric measurements shows a good quality of the manufactured coils and quadrupole lenses.

Taking into account the recommendations of the 21-st. session of PAC for nuclear physics, the IREN project leaders proposed to prolong theme 06-4-0993-94/2004 for one year with top priority. The main tasks to be implemented in the course of 2005 are:

- completion of the dismantling of the IBR-30 reactor and preparation for receiving the license for the IREN construction;
- receiving of the design documentation for the multiplying target from NIKIET and choosing of its producers with the aim of real estimation of the final cost of the IREN project;
- detail designing of the IREN backup systems in the amount necessary for the assembling of the equipment of the linac LUE-200;
- completion of the assembling of the main equipment of the linac LUE-200 in bldg.43, FLNP.

The realization requires financing which would not exceed the average annual funding of the IREN project and the total budget of theme 06-4-0993-94/2005. The execution of the stated tasks can be considered as a basis for making strategic decisions on the project future.

2. НЕЙТРОННЫЕ ИСТОЧНИКИ

2.1. Импульсный реактор ИБР-2

В 2004 г. ИБР-2 отработал на физический эксперимент ~ 1384 час (см. **таблицу 1**).

Таблица 1

Эксплуатационные показатели работы реактора ИБР-2 в 2004 г.

№ цикла	**1**	**2**	**3**	**4**	**ВСЕГО:**
Время цикла	13.09 - 24.09	18.10 - 05.11	15.11 - 26.11	06.12 - 24.12	
1. Наработка на физический эксперимент, час	264	418	268	434	**1384**
2. Наработка ПО-3, час	273	434	275	443	**1425**
3. Энергонаработка, МВт·час	402	633	404	653	**2092**
4. Количество срабатываний аварийной защиты (АЗ)	1	2	–	–	**3**
5. Причины срабатываний АЗ:					
5.1. Посадки напряжения	–	2	–	–	**2**
5.2. Неисправности и отказы оборудования	1	–	–	–	**1**
5.3. Сбои в электронной аппаратуре	–	–	–	–	**–**
5.4. Ошибки персонала	–	–	–	–	**–**

Основные результаты по модернизации ИБР-2 в 2004 г.:

1) ПО-3 – главная задача года.

В начале февраля 2004 г. полностью завершена сборка ПО-3 на стенде ЛНФ и осуществлен пуск на номинальных оборотах (**рис.1**). Выполнена программа исследований ПО-3 в режимах 5 и 10 Гц по измерению вибрационных характеристик. Все параметры ПО-3 соответствуют техническим требованиям. Также проведены ресурсные испытания, которые не выявили каких-либо отклонений в работе ПО-3, все системы работали штатно. Далее машина была перевезена в здание реактора.

Выполнен монтаж ПО-3 на штатном месте около реактора, проведены испытания, ПО-3 принят в эксплуатацию ГАН.

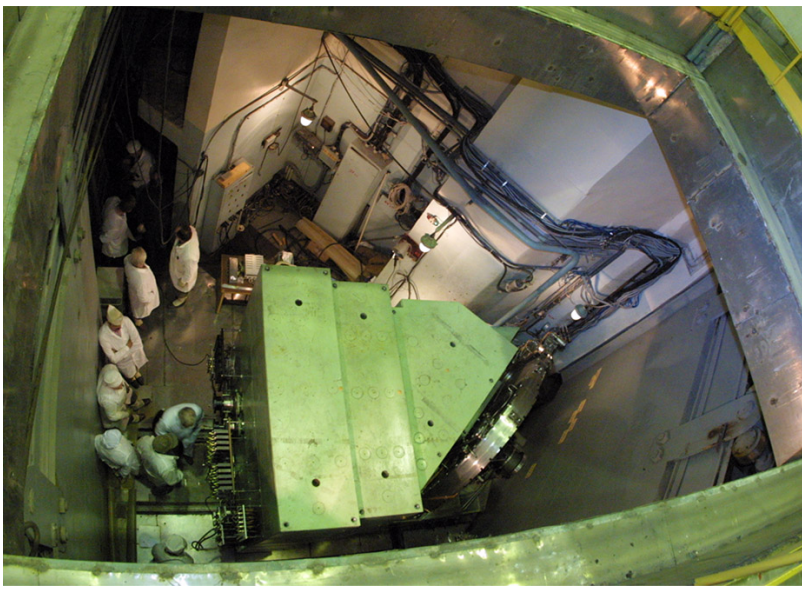

Рис. 1. *ПО-3 перед установкой на штатное место.*

С 16.06.2004 г. по 23.07.2004 г. выполнена Программа пуска и исследования основных характеристик ИБР-2 с новым ПО-3: измерена кривая эффективности подвижного отражателя в стационарном режиме, (см. **рис. 2**) измерены эффективности блоков регулирования, определен оперативный запас реактивности, произведена догрузка реактора одной ТВС, измерены форма импульса и флуктуации импульсов до 1,5 МВт. Полученные результаты близки к расчетным (см. **рис. 3, 4**).

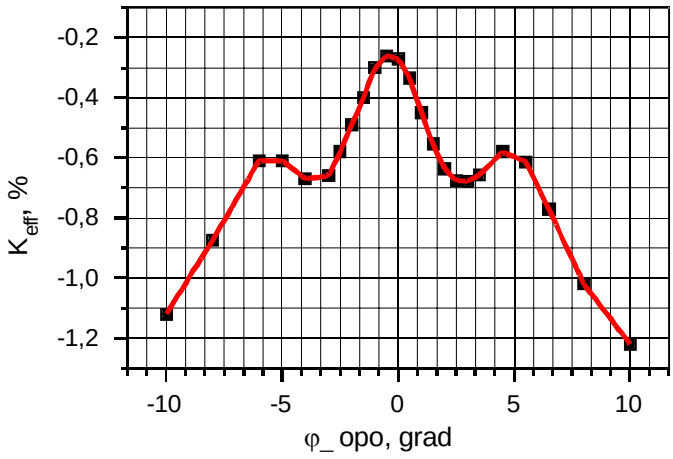

Рис. 2. *Ход реактивности при смещении роторов ПО-3 в интервале ± 10 градусов ОПО. По оси абсцисс – смещение ОПО в градусах, по оси ординат – отклонение коэффициента размножения от единицы.*

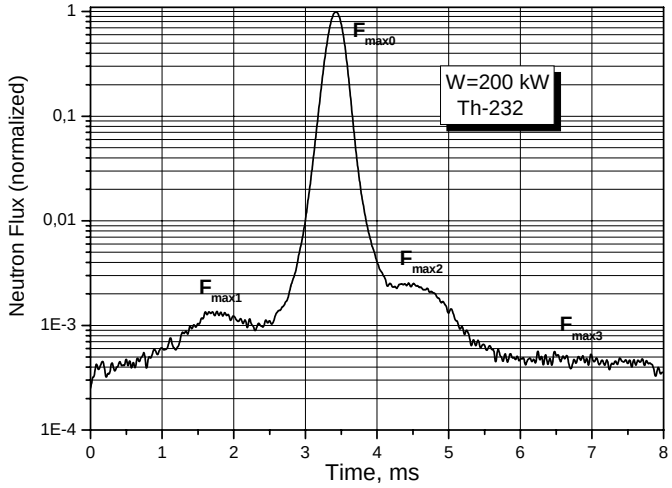

Рис. 3. *Форма импульса мощности. Данные нормированы на максимум импульса. Измерения с помощью Th-232 - камеры.*

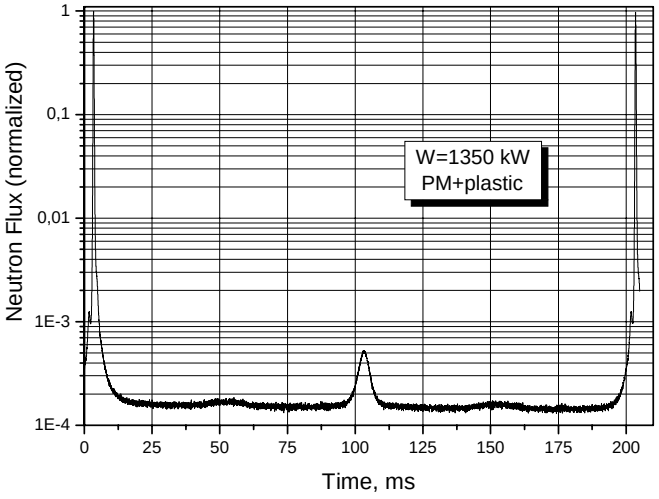

Рис. 4*. Распределение мощности между двумя последовательными вспышками. Данные нормированы на максимум вспышки. Измерение с помощью сцинтилляционного детектора.*

Таким образом, завершен очень важный этап модернизации ИБР-2 по созданию нового ПО-3.

С 13.09.2004 г. началась плановая работа на физический эксперимент в соответствии с графиком.

2) На ПО «Маяк» завершено изготовление ТВЭЛ. В апреле 2004 г. ТВЭЛы были доставлены в ОИЯИ. Ведутся работы по подготовке участка для сборки ТВЭЛ в ТВС.
3) Завершены работы по выпуску конструкторской документации на стационарные отражатели и откатные защиты.
4) Продолжалось изготовление в НИКИЭТ нового корпуса реактора, развернуто изготовление откатных защит и стационарных отражателей в ОП ОИЯИ.
5) Продолжалась разработка конструкторской документации (КД) по СУЗ ИБР-2.

На обеспечение работ по модернизации ИБР-2 в 2004 г. было израсходовано 696 k$, в т.ч. ОИЯИ – 348 k$, Федеральное агентство по атомной энергии – 348 k$.

«Разработка комплекса замедлителей нейтронов широкого спектра («комби-замедлителей») для модернизируемого исследовательского реактора ИБР-2М»

1. Изготовлена установка и проведены эксперименты по измерению давления водорода в камере замедлителя с мезитиленом при облучении в условиях, имитирующих рабочие (на микротроне МТ-25 ЛЯР). В результате анализа получено, что в проектируемом холодном замедлителе на основе мезитилена максимальное давление на оболочку при отогреве мезитилена может достигнуть 25 бар после суток работы. Этот результат дает исходные данные для выбора параметров твэла замедлителя. Подготовлена рукопись для публикации в виде сообщения ОИЯИ.
2. Закончена разработка оптимальной конфигурации замедлителей на направлении 4, 5, 6, 1 и 9-го пучков (**рис.5**), а также 2-го и 3-го пучков. Расчетным путем получены значения спектральной плотности потоков нейтронов (**рис.6**), которые в области коротких волн значительно выше, а в области холодных нейтронов находятся на уровне проектируемого твердометанового замедлителя второй мишени источника ISIS. Таким образом, вместе с ранее сделанной оптимизацией комби-замедлителей для пучков 7-го, 8-го, 10-го и 11-го, композиция всего комплекса замедлителей разработана. Готовится текст доклада на международную конференцию ICANS XVII, США, апрель 2005.
3. Разработан принцип трубной конструкции мезитиленового холодного замедлителя, обеспечивающий, как минимум, не менее чем 3-4 суточную непрерывную работу без отжига водорода и длительный общий ресурс работы в условиях ИБР-2М. Имеется публикация – Е.П. Шабалин, С.А. Куликов. Сообщение ОИЯИ, Р13-2004-73.
4. Составлено техническое задание на проектирование комплекса замедлителей совместно с НИКИЭТ.
5. Начаты лабораторные эксперименты по поиску методики приготовления шариков твердого мезитилена диаметром 10-15 мм. В случае положительного результата конструкция замедлителя может быть более простой, более дешевой в изготовлении и удобной в эксплуатации.

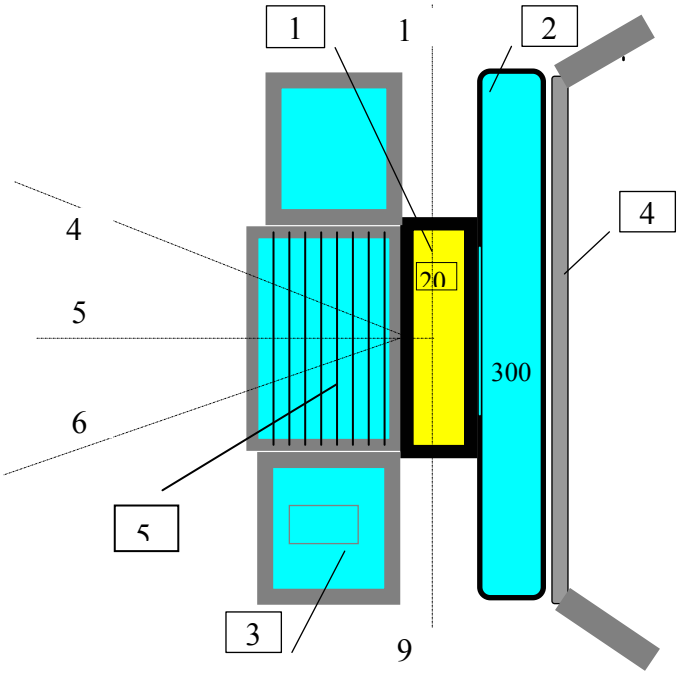

Рис.5. *1- холодный замедлитель; 2 – предзамедлитель; 3- плоский пост-замедлитель; 4- граница реактора; 5 – гребенчатый пост-замедлитель.*

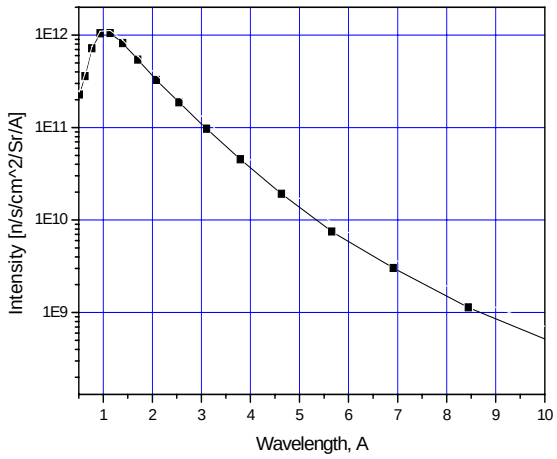

Рис.6. *Дифференциальная плотность потока нейтронов с торцов холодного замедлителя (направление пучков 1 и 9).*

Планы на 2005 г.

1. Сборка ТВЭЛов в тепловыделяющие сборки (ТВС).
2. Продолжение работ по изготовлению нового корпуса реактора и другого основного оборудования.
3. Разработка электронной аппаратуры СУЗ ИБР-2М и исполнительных механизмов СУЗ.
4. Разработка технического проекта комплекса замедлителей для ИБР-2М.
5. Изготовление ХГУ.

2.2. Проект ИРЕН

План работ по проекту ИРЕН на 2004 год содержал следующие основные задачи:

1. завершение демонтажа реактора ИБР-30;
2. доставка топлива размножающей мишени из ПО «Маяк» в ОИЯИ;
3. монтаж основного оборудования ускорителя ЛУЭ-200 в зд. 43.

Объем минимального финансирования для реализации этого плана составлял 250 тыс. долл. США. Реально в марте 2004 года. было выделено около половины необходимой суммы с гарантиями оплаты только первых двух задач. К тому же значительные средства (около 50 тыс. долл. США) необходимо было затратить для выплаты долга НИКИЭТ за выполненную в течение 2002-2003 гг. работу по подготовке конструкторской документации для изготовления размножающей мишени ИРЕН.

До середины августа план-график работ по демонтажу реактора ИБР-30 выполнялся с небольшими задержками, несмотря на очень трудную ситуацию с наполнением бюджета ОИЯИ. Но 19.08.04 вступило в действие постановление Правительства РФ о реорганизации Госатомнадзора и Министерства экологии, что привело к приостановке рассмотрения заявок на лицензирование деятельности в области использования атомной энергии. Это вызвало существенную задержку в получении лицензии на ввод в эксплуатацию здания 117/6-хранилища активированных элементов конструкции реактора ИБР-30 и, фактически, исключило возможность завершения работ по демонтажу реактора в 2004 году, как это было запланировано.

Переговоры с представителями реорганизуемого Ростехнадзора, включающего в качестве управления прежний Госатомнадзор, показывают, что необходимые лицензии могут быть получены в первом квартале 2005 года, и, соответственно, работы по демонтажу

реактора смогут проводиться в течение лета будущего года. Важно отметить, что все работы из плана-графика 2004 года, которые должны были выполняться службами ЛНФ, успешно завершены.

Большой объем работ был выполнен по подготовке к транспортировке топлива для размножающей мишени ИРЕН. 8 декабря 2004 г. транспортировка топлива из ПО «Маяк» в ОИЯИ завершена.

В связи с практическим отсутствием финансирования работ по монтажу оборудования ускорителя ЛУЭ-200 эти работы велись в основном за счет внутренних резервов. Однако определенный прогресс был достигнут в создании электронного источника, элементов фокусирующей и ВЧ систем. Импульсная электронная пушка была доведена до проектных параметров, что было подтверждено ее успешным испытанием. Основное оборудование ВЧ модулятора было установлено на штатном месте в ускорительном зале зд. 43 ЛНФ. На полномасштабном ВЧ стенде была успешно испытана система удвоения мощности питания клистрона. Однако отсутствие средств на приобретение необходимых кабелей и ряда комплектующих привело к задержке запланированного завершения монтажа основного оборудования ускорителя ЛУЭ-200.

Изготовление элементов магнитной фокусирующей системы в ЛФЧ и ЛВЭ было остановлено в сентябре из-за отсутствия финансирования. К настоящему времени изготовлено около 70% всей фокусирующей системы. Испытание ее элементов на недавно созданном магнитометрическом стенде ЛФЧ показало высокое качество изготовления катушек соленоида и квадрупольных линз.

Учитывая рекомендации 21-й сессии ППК по ядерной физике руководство проекта ИРЕН предложило продлить тему 06-4-0993-94/2004 на один год с первым приоритетом. Главными задачами, которые должны быть выполнены в течение 2005 года, являются:

- завершение демонтажа реактора ИБР-30 и подготовка к получению лицензии на строительство установки ИРЕН;
- получение из НИКИЭТ конструкторской документации размножающей мишени и выбор ее изготовителей с целью реальной оценки стоимости завершения проекта ИРЕН;
- рабочее проектирование вспомогательных систем ИРЕН в объеме необходимом для монтажа основного оборудования ускорителя ЛУЭ-200;
- завершение монтажа оборудования ЛУЭ-200 в зд. 43 ЛНФ.

Реализация этого плана требует средств, не превышающих среднее ежегодное финансирования проекта ИРЕН и полный бюджет темы 06-4-0993-94/2005. Выполнение сформулированных задач может рассматриваться как основа для принятия стратегических решений о будущем проекта ИРЕН.

3. DEVELOPMENT AND CREATION OF ELEMENTS OF NEUTRON SPECTROMETERS FOR CONDENSED MATTER INVESTIGATIONS

In 2004 work under theme 1052 was focused on the following main activities:

- creation of neutron detectors;
- development of sample environment systems;
- development of data acquisition systems and computing infrastructure.

1. Creation of neutron detectors

1.1.Infrastructure

To provide necessary conditions for manufacturing and testing of the different types of neutron PSDs, a clean room has been put into service in FLNP. It consists of three parts: a tambour, clean room and a clean box inside the clean room. At present, the air purity in the clean room is better than class 7 according to ISO 14644-1 standard, which is enough to assembly gas MWPC. For assembling microstrip detectors a laminar cabinet will be used (shipped to Dubna in October 2004 and being assembled now).

A gas stand has been put into use, allowing oil-free pumping out of the detector chambers and filling them with various gas mixtures under pressure. The gas stand together with other technological equipment is placed in the tambour of the clean room (**Fig.1,2**).

Fig.1*. Vacuum furnace, water purifying system and ultrasonic bath.*

Fig.2*. Gas-filling system.*

In cooperation with specialists from IPM RAS (Nizhni Novgorod) the wire winding system (based on comb-like spacers made of siliceous monocrystal) for manufacturing multiwire proportional chambers has been significantly improved. This has been achieved by the use of spacers made of silicon monocrystals, where grooves for laying wires are etched with a high degree of accuracy (several microns). The system will be used to produce anode and cathode planes for a position-sensitive monitor and 1D detectors.

1.2.Microstrip neutron detector with "virtual" cathode

In cooperation with the detector group of the Institute Laue-Langevin a Microstrip Gas Counter (MSGC) has been created using the "virtual" cathode technology. The drawings of the substrate plate were placed at our disposal by ILL, substrate plates were manufactured at IPM RAS

(Nizhni Novgorod, Russia) and successfully tested at ILL last year. The original design of the detector case was developed and manufactured at FLNP.

The first results of the detector testing with a ^{252}Cf neutron source are shown in Figs.3,4. **Figure 3** illustrates the result of uniform irradiation of the detector for 1 coordinate. In **Fig.4** the result of irradiation of the detector with a collimation mask made of borated polyethylene (5 cm thick with two 5 mm slits at 10 mm distance) is presented. The geometrical dimensions of the slit images on the detector plane were 10 mm. The gas mixture (1 bar) consisted of ^{3}He (0.5 bar) and CF_4 (0.5 bar), so the coordinate resolution was only 5 mm. At a working pressure of 2 bar of CF_4 the coordinate resolution is expected to be 1.5 mm.

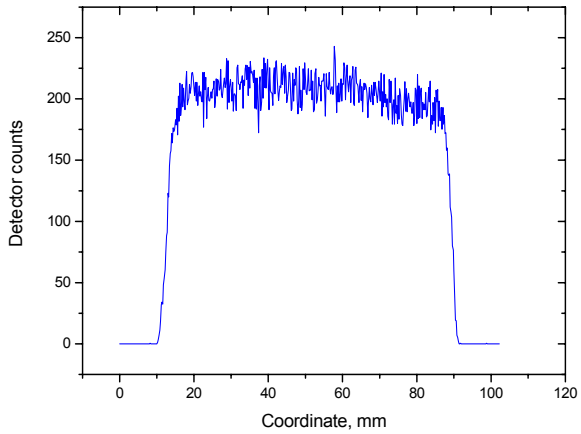

Fig.3. *Uniform distribution for 1 coordinate.*

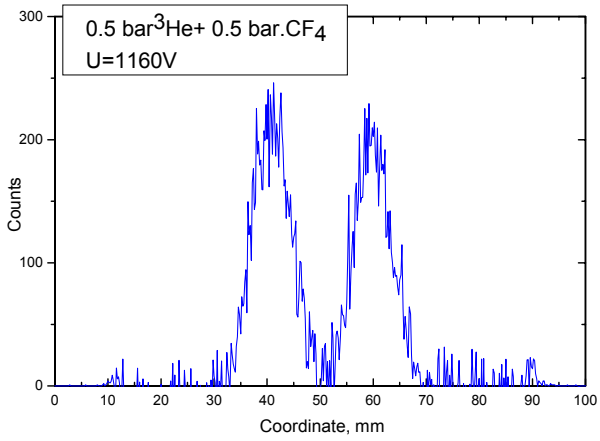

Fig.4. *One coordinate image of two slits in the collimation mask.*

1.3. Prototype of one-dimensional PSD for the Fourier Stress Diffractometer

The design of a 1D wide-aperture neutron PSD has been developed at FLNP. The detector parameters are listed in **Table 1**.

Parameter	Value
Aperture	200 x 80 mm^2
Position resolution (FWHM)	Δx = 1.5 mm (centre)
Efficiency (1 Å)	40-45%
Detector count rate	R up to 100 kHz
Readout	Delay line
Gas mixture	^{3}He + 0.25 CF_4 (6 atm)

At the present time the manufacturing of the detector case is being completed in the central JINR workshops. The assembling and beam tests at the IBR-2 reactor are scheduled for the beginning of 2005. A similar detector will be produced next year for the Institute of Metal Physics, of the RAS Ural Branch (Yekaterinburg) under the contract in force.

1.4. Position-sensitive monitor detector

Within collaboration between FLNP and Technical University of Munich the specifications on an in-beam position-sensitive monitor have been prepared. The detector is to be installed on a bent neutron guide outside the reactor hall of the FRM-II reactor. The detector will be a multiwire proportional chamber with a ^{3}He gas mixture. The main features of the detector are listed in **Table 2**.

Parameter	Value
Sensitive area	100 x 100 mm^2
Position resolution (FWHM)	$\Delta x \approx 4$ mm $\Delta y \approx 4$ mm
Sensitivity for thermal neutrons	$S_{th} = 10^{-3} – 10^{-6}$
Range of neutron wavelengths	$\lambda = 0.4$ Å – 12 Å
Detector count rate	R = 1 kHz – 50 kHz
Readout	Delay lines

At present the manufacturing of the detector main units is being completed at the central JINR workshops. Beam tests at IBR-2 and later at FRM-II are scheduled for the beginning of 2005. **Figure 5** shows the detector box and electrode frames.

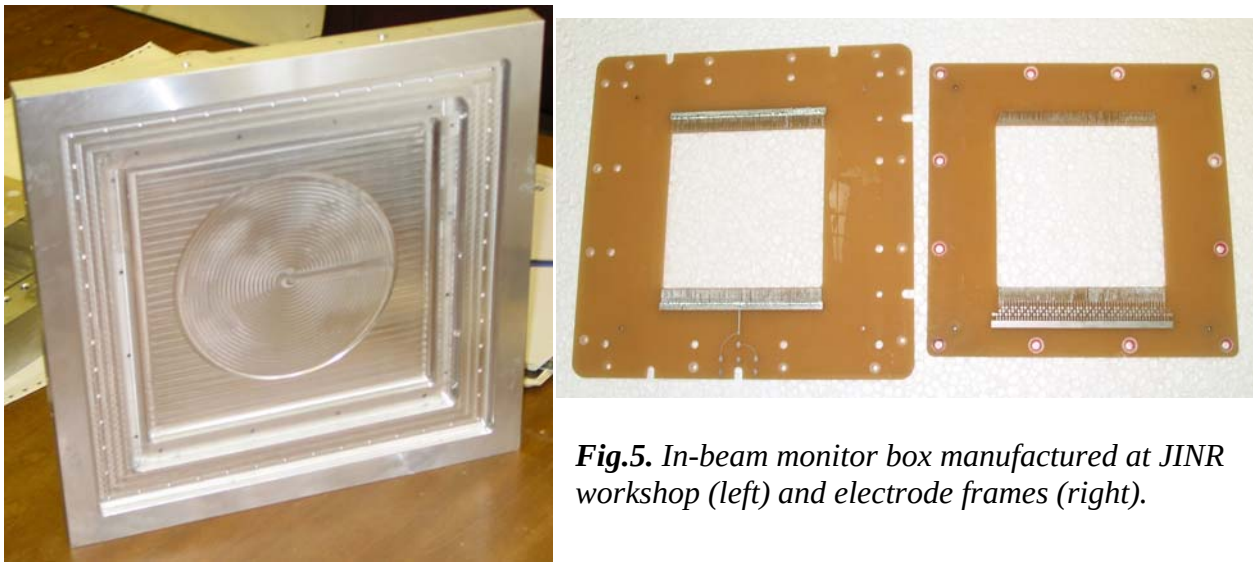

Fig.5. *In-beam monitor box manufactured at JINR workshop (left) and electrode frames (right).*

1.5. Scintillation detectors

For the FSD spectrometer 16 additional modules of the 90° scintillation detector with the ASTRA time focusing have been developed and manufactured (**Fig.6**). The detector electronics units have been made. The mechanical units for fixing the detector modules have been manufactured. At present the detectors are being assembled and tested.

Calculations have been made by the method of focusing surfaces of the geometry of detector sensitive layers to detect neutrons at scattering angles of 90° and 45°. For the DN-6 spectrometer it is proposed to produce a detector consisting of two rings. Each ring consists of 16 independent modules. The designs of the detector modules for both rings have been worked out, as well as the support of the detector modules. The project is submitted for approval by experimenters.

Fig.6. *Module of the 90^0 scintillation detector with the ASTRA time focusing.*

2. Development of sample environment systems

A temperature control system has been developed on the basis of a Eurotherm 902 controller for the equipment of the Epsilon spectrometer.

To adjust the monochromator (Si-monocrystal with a bending device, made in NPI Rez, Czech Republic for the DSD spectrometer of the IVV-2M reactor of Sverdlovsk branch of A.N.Dollezhal Research and Development Institute of Power Engineering) a goniometric device with 5 degrees of freedom (two swinging motions and two linear motions in mutually perpendicular directions and rotation around a vertical axis) has been manufactured. (**Fig.7**).

Fig.7. *Monochromator with a goniometric device.*

For the DSD spectrometer a control system for mechanical devices has been made as well. The control system is realized in CAMAC standard with a microcontroller control block for SMC step motors on the basis of a 80C167 microprocessor connected to a personal computer via a serial communication line. Four-channel commutators-amplifiers SMD-2A are used as a power drive of 4-phase step motors (a total of 18). The system can be extended by connecting SMD-2A additional blocks to the SMC controller.

The range of functions of the control system of the step motors of the SPN spectrometer has been extended (neutron guide platform movement, control over a two-coordinate diaphragm, as well as over rotating actuators).

A positioning device with 3 degrees of freedom has been manufactured for a variable diaphragm of the neutron beam of the HRFD spectrometer (Fig.8). Control is exercised via the

control system of the Huber goniometer.

Fig.8. *Variable diaphragm with a positioning device.*

On the Isomer spectrometer the chopper control system on the basis of the microcontroller control unit CC-11 has been put into operation. The phase equalization accuracy is 25-30 μs. If the phase goes beyond a specified range, the measurement is interrupted by blocking reactor starts in the "KOMA" spectrometric data accumulation system.

The design documentation for a cryostat with a refrigerator based on the pulse tubes PT405 (Cryomech, USA) for operation in the temperature range of 250-3 K has been worked out. At the present time the cryostat components are being manufactured in the FLNP experimental workshops. Such a cryostat with a refrigerator based on pulse tubes is made for the first time in Russia.

A sorption pumped microrefrigerator to obtain temperatures down to 0.3 K has been designed. The microrefrigerator is mounted on a platform having a temperature of 4.2 K, which can be obtained in an ordinary helium cryostat or by means of an appropriate closed cycle refrigerator. In our case the microrefrigerator is installed at the bottom of a helium optical cryostat. This work has been carried out in cooperation with the Institute of Radioelectronics RAS (Moscow) and the Institute of Applied Physics RAS (Nizhni Novgorod).

3. Development of data acquisition systems and computing infrastructure

In 2004 in the frame of works to integrate PC into DAQ systems the creation of the new unified instrument control software Sonix+ was completed. The VME/OS-9 platform has been replaced with PC/Windows with Python being used as a script language. The use of PC with Windows OS for instrument control reduces the overall cost of the system. The existing VME electronics can be connected to PC via a VME-PCI adapter. Due to the structural changes the Sonix+ software package has become more powerful, flexible and simple for users and, at the same time, more unified and easily extendable.

At the moment the Sonix+ successfully operates on the NERA-PR spectrometer. The extended version of the Sonix+ for the REMUR and YuMO spectrometers is in the final stage of testing.

The software for a delay line readout PCI DAQ board (FPGA, DSP and PC components) for MWPC detectors has been tested and optimized to enhance reliability and acquisition rate up to 10^6 events per second.

An analysis of engineering solutions for MSGC DAQ electronics with individual strip readout has been performed. As a result, it was decided to order two-coordinate electronics for charge division readout (designed at ILL) from the SYNERGIECONCEPT Company (Grenoble,

France). The USB interface for this electronics and corresponding software is to be designed at FLNP.

In the LAN segment of the experimental halls of the IBR-2 reactor two Switch Catalist 2950C-24 together with Uninterrupted Power Supplies have been installed and put into operation. The modernization of the power supply system of electronics and computers has been performed for the YuMO and FSD spectrometers as well.

The development of new electronic blocks with USB interfaces for data acquisition systems of point detectors and multiwire PSDs with individual data readout from each wire has been started.

A number of detector electronics blocks have been developed, manufactured, tested and put into operation on the IBR-2 spectrometers.

Through the reported year the equipment of the spectrometers has been prepared for operation and serviced during a total of 4 cycles of the IBR-2 reactor.

3. РАЗРАБОТКА И СОЗДАНИЕ ЭЛЕМЕНТОВ НЕЙТРОННЫХ СПЕКТРОМЕТРОВ ДЛЯ ИССЛЕДОВАНИЯ КОНДЕНСИРОВАННЫХ СРЕД

Работы по теме велись в следующих основных направлениях:
- создание нейтронных детекторов;
- развитие систем окружения образца;
- развитие систем сбора данных и вычислительной инфраструктуры.

1. Создание нейтронных детекторов

1.1 Инфраструктура

Для обеспечения необходимых условий при изготовлении и тестировании различных типов позиционно-чувствительных детекторов (ПЧД) была создана и введена в эксплуатацию «чистая комната». Она состоит из трех частей: тамбура, собственно чистой комнаты и чистого бокса внутри нее. В настоящее время чистота воздуха в чистой комнате превышает класс 7 согласно стандарту ISO 14644-1, что достаточно для сборки газовых MWPC детекторов. Для сборки микростриповых детекторов будет использоваться ламинарный бокс (поставлен в Дубну в октябре 2004г. и сейчас находится в монтаже).

Создан газовый стенд, позволяющий производить откачку газа из камер детекторов и заполнять их различными смесями газов, в том числе и под давлением. Газовый стенд вместе с другим технологическим оборудованием смонтирован в тамбуре чистой комнаты (**Рис.1,2**).

Рис.1. *Вакуумная печь, система очистки воды и ультразвуковая печь*

Рис.2. *Газовый стенд*

Совместно со специалистами ИФМ РАН (Н.Новгород) значительно улучшена система намотки нитей в многопроволочных пропорциональных камерах. Это достигнуто за счет применения спейсеров из монокристаллов кремния, в которых с высокой точностью (несколько микрон) протравлены канавки для укладки нитей. Новая система будет использоваться для изготовления анодных и катодных плоскостей ПЧД монитора и однокоординатных детекторов.

1.2 Микростриповый нейтронный детектор с «виртуальным» катодом

В сотрудничестве с детекторной группой Института Лауэ-Ланжевена (Гренобль) был создан микростриповый газовый детектор (MSGC), использующий технологию «виртуального» катода. Рисунки микростриповых структур были представлены нам ИЛЛ, сами подложки были изготовлены в ИФМ РАН и затем успешно испытаны в ИЛЛ. Оригинальный корпус детектора был разработан и изготовлен в ЛНФ.

Первые результаты тестирования детектора с источником ^{252}Cf показаны на рисунках 3,4. **Рис.3** иллюстрирует результат равномерного облучения детектора по одной координате. На **Рис.4** показан результат облучения детектора с коллимационной маской, изготовленной из борированного полиэтилена (толщина маски 5см, в ней вырезаны две щели по 5мм, расположенные на расстоянии 10мм). Геометрические размеры изображения щелей на плоскости детектора составляли 10мм. Газовая смесь (1 бар) состояла из ^{3}He (0,5 бар) и CF_4 (0,5 бар), так что координатное разрешение было только 5мм. При рабочем давлении 2 бара CF_4 ожидается улучшение разрешения до 1,5мм.

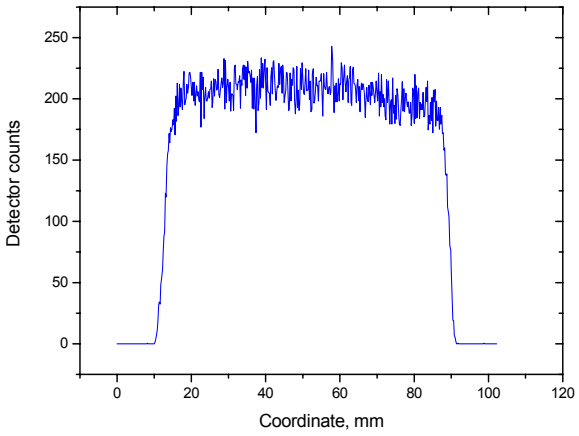

***Рис.3**. Равномерное распределение по одной координате*

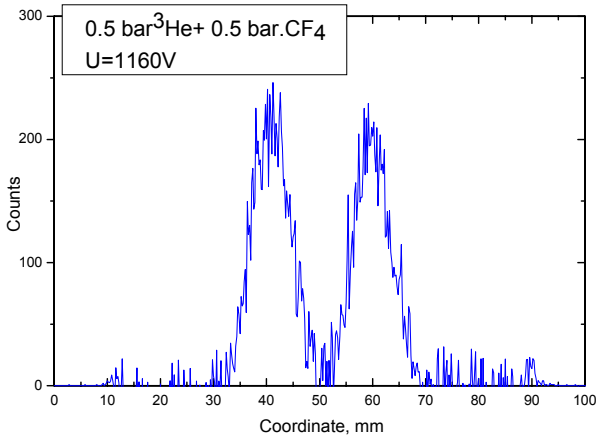

***Рис.4.** Изображение двух щелей в коллимационной маске по одной координате*

1.3. Прототип однокоординатного ПЧД для дифрактометра ФСД

Разработан проект 1D широкоапертурного ПЧД, его параметры показаны в **таблице 1.**

Параметр	Величина
Апертура	200 x 80 mm^2
Позиционное разрешение (FWHM)	Δx = 1.5 mm (centre)
Эффективность(1 Å)	40-45%
Скорость счета	R up to 100 kHz
Метод считывания	Линия задержки
Газовая смесь	^{3}He + 0.25 CF_4 (6 atm)

В настоящее время завершается изготовление корпуса детектора в Опытном производстве ОИЯИ. Сборка и тестирование на пучке ИБР-2 планируется в начале 2005г. Аналогичный детектор будет изготовлен также для Института физики материалов УО РАН (Екатеринбург) по действующему контракту.

1.4.Позиционно-чувствительный мониторный детектор

В рамках коллаборации ЛНФ и Технического Университета, Мюнхен разработан технический проект и детальная спецификация двухкоординатного позиционно-чувствительного монитора нейтронного пучка. Монитор планируется установить на изогнутом нейтроноводе вне реакторного зала реактора FRM-II. Детектор будет представлять собой многопроволочную пропорциональную камеру с газовой смесью на основе ^{3}He. Основные характеристики детектора перечислены в **таблице 2.**

Параметр	**Величина**
Чувствительная область	100 x 100 mm^2
Позиционное разрешение (FWHM)	$\Delta x \approx 4$ mm $\Delta y \approx 4$ mm
Чувствительность к тепловым нейтронам	$S_{th} = 10^{-3} – 10^{-6}$
Диапазон длин волн	$\lambda = 0.4$ A – 12 $\oplus$
Скорость счета	R = 1 kHz – 50 kHz
Метод считывания	Линии задержки

В настоящее время в ОП ОИЯИ завершается изготовление основных узлов детектора. Тестовые испытания на пучке ИБР-2, а затем на реакторе FRM-II, планируются в первой половине 2005г. На **Рис.5** показаны корпус детектора и электродные плоскости.

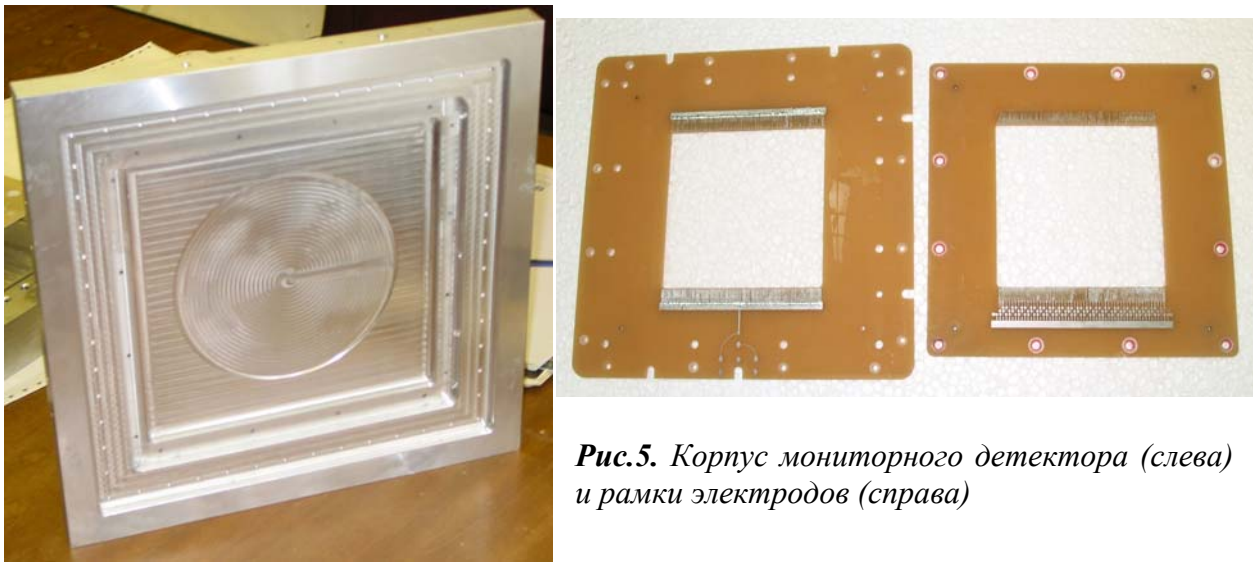

Рис.5. *Корпус мониторного детектора (слева) и рамки электродов (справа)*

1.5. Сцинтилляционные детекторы

Для спектрометра ФСД разработаны и изготовлены 16 дополнительных модулей 90^0 сцинтилляционного детектора с временной фокусировкой АСТРА (**Рис.6**). Изготовлены узлы детекторной электроники. Изготовлены механические узлы фиксации детекторных модулей. В настоящее время проводится сборка и испытания детекторов.

Рис.6. *Модуль 90^0 сцинтилляционного детектора с временной фокусировкой ASTRA.*

Проведены расчеты по методу фокусирующих поверхностей геометрии чувствительных слоев детектора для регистрации нейтронов на углах рассеяния 90 и 45 градусов. Для спектрометра ДН-6 предполагается изготавливать детектор, состоящий из двух колец. Каждое кольцо составлено из 16 независимых модулей. Разработаны конструкции отдельных модулей детектора для обоих колец. Разработана конструкция поддержки модулей детектора. Проект находится в стадии согласования с экспериментаторами.

2.Развитие систем окружения образца

Разработана система регулирования температуры на базе контроллера Eurotherm 902 для комплекса оборудования спектрометра Эпсилон.

Для юстировки монохроматора (Si-монокристалл с изгибателем, изготовленный в ИЯФ г.Ржеж ЧР для спектрометра ДСД реактора ИВВ-2М Свердловского филиала НИКИЭТ) изготовлено гониометрическое устройство, имеющее 5 степеней свободы (два качания и два линейных перемещения во взаимно-перпендикулярных направлениях и вращение вокруг вертикальной оси) (**Рис.7**).

Рис.7. *Монохроматор с гониометрическим устройством.*

Для спектрометра ДСД изготовлена также система управления механическими устройствами. Система управления реализована в стандарте КАМАК с микроконтроллерным блоком управления шаговыми двигателями SMC на базе микропроцессора 80C167, подключенного к персональному компьютеру по последовательной линии связи. В качестве силового привода 4-х фазных шаговых двигателей (общее количество 18) используются

четырехканальные коммутаторы-усилители SMD-2A. Система может быть расширена подключением к контроллеру SMC дополнительных блоков SMD-2A.

В состав системы управления исполнительными механизмами спектрометра СПН добавлено перемещение платформы нейтроновода, управление двухкоординатной диафрагмой, а также управление поворотными исполнительными механизмами.

Для регулируемой диафрагмы рассеянного пучка нейтронов спектрометра ФДВР изготовлено юстировочное устройство, имеющее 3 степени свободы (**Рис.8.**). Управление осуществляется через систему контроля гониометра Huber.

Рис.8. *Регулируемая диафрагма с юстировочным устройством.*

На спектрометре Изомер введена в эксплуатацию система управления прерывателем на базе микроконтроллерного блока управления СС-11. Точность стабилизации фазы составила 25-30 мкс. При выходе фазы из заданного диапазона, измерения приостанавливаются путем блокировки стартов реактора в системе накопления спектрометрической информации «КОМА».

Разработана конструкторская документация на криостат с рефрижератором на импульсных трубках РТ405 (Cryomech, USA) для работы в диапазоне температур 250–3 К. В настоящее время детали криостата изготавливаются в экспериментальных мастерских ЛНФ. Криостат с рефрижератором на импульсных трубках изготавливается впервые в России.

Разработан микрорефрижератор с сорбционной откачкой (**Рис.9.**) для получения температур до 0.3 К. Микрорефрижератор устанавливается на платформу, имеющую температуру 4.2 К, которая может быть получена в обыкновенном гелиевом криостате или при помощи подходящего рефрижератора замкнутого цикла. В нашем исполнении микрорефрижератор устанавливался на дно гелиевого оптического криостата. Данная работа выполнена в сотрудничестве с Институтом радиоэлектроники РАН (Москва) и Институтом прикладной физики РАН (Нижний Новгород).

Рис.9. *Микрорефрижератор с сорбционной откачкой для получения температур до 0.3 К.*

3.Развитие систем сбора данных и вычислительной инфраструктуры

В рамках работ по интеграции PC в системы сбора данных в 2004г. завершено создание нового унифицированного программного комплекса Sonix+ для управления оборудованием спектрометров и экспериментом. Платформа VME/OS-9 была заменена на платформу PC/Windows и Python был использован как язык описаний. Существующая VME электроника подключается к PC через VME-PCI адаптеры. Благодаря структурным изменениям комплекс Sonix+ стал более мощным, гибким и простым в применении и в то же время более универсальным и легко расширяемым. Переход на платформу PC/Windows уменьшает общую начальную стоимость систем автоматизации спектрометров и, что особенно важно, существенно снизит затраты на модернизацию и развитие этих систем в будущем.

В настоящее время Sonix+ успешно эксплуатируется на спектрометре HEPA-ПР. Расширенные версии Sonix+ для спектрометров РЕМУР и ЮМО находятся в завершающей стадии тестирования.

Программное обеспечение (FPGA, DSP и PC компоненты) платы сбора данных для MWPC детекторов с линиями задержки было переработано и оптимизировано с целью повышения надежности и увеличения скорости накопления данных до 10^6 соб/с.

Проведен анализ технических решений DAQ электроники для MSGC детектора с индивидуальным считыванием информации с каждого стрипа. В результате решено приобрести комплект DAQ электроники, разработанный в ИЛЛ и производящейся фирмой Synergieconcept (Гренобль). USB интерфейс для этой электроники будет разработан в ЛНФ.

В LAN сегменте экспериментальных залов ИБР-2 установлены два новых сетевых коммутатора Catalyst 2950C-24 вместе с источниками бесперебойного питания. Модернизация системы электропитания электроники и компьютеров выполнена также на спектрометрах ЮМО и ФСД.

Начата разработка новых электронных блоков с USB интерфейсом для накопления данных от точечных детекторов и многопроволочных ПЧД с индивидуальным считыванием информации с каждой нити.

Выполнены разработки ряда блоков детекторной электроники, в течение года они были изготовлены, протестированы и установлены на спектрометрах ИБР-2.

В текущем году были полностью обеспечены подготовка оборудования спектрометров к четырем циклам реактора, а также электронная и компьютерная поддержка экспериментов.

4. EXPERIMENTAL REPORTS

4.1. CONDENSED MATTER PHYSICS

Diffraction

Comparative Study of the Magnetic Phase Diagrams of Nearly Half-Doped $Sm_{1-x}Sr_xMnO_3$ with ^{16}O and ^{18}O Isotopes
A.M.Balagurov, N.A.Babushkina, E.A.Chistotina, I.A.Bobrikov, V.Yu.Pomjakushin, A.I.Kurbakov, V.A.Trunov, O.Yu.Gorbenko, A.R.Kaul, K.I.Kugel

Crystal Structure of Lithium Beryllium Deuteride Li_2BeD_4
B.M.Bulychev, R.V.Shpanchenko, E.V.Antipov, D.V.Sheptyakov, S.N.Bushmeleva, A.M.Balagurov

Pressure Induced Phase Ytansition in Ferroelectric Pirydinium Perrhenate
P.Czarnecki, A.I.Beskrovny, L.Bobrowicz-Sarga, S.Lwicki, J.Wasicki

Temperature- and Composition-Driven Changes of Magnetic Moments and Lattice Parameters in Quasibinary $(Sc_{1-x}Y_x)Fe_2$ Laves Phase Compounds
Z.Surowiec, A.I.Beskrovnyi, M.Wiertel, J.Sarzynski, M.Budzynski

Neutron Study of $Mn_3Fe_4V_6O_{24}$
N.Guskos, A.Beskrovnyi, J.Typek, N.Yu.Ryabova, A.Blonska-Tabero, M.Kurzawa, M.Maryniak

High Pressure Effects on the Crystal and Magnetic Structure of $Pr_{1-x}Sr_xMnO_3$ Manganites (x=0.48, 0.85)
D.P.Kozlenko, V.P.Glazkov, Z.Jirak, B.N.Savenko, S.E.Kichanov

Inelastic Scattering

IINS and NMR Study of 11 Keto Progesterone
K.Holderna-Natkaniec, I.Natkaniec, A.Szyczewski

Microscopic Structure of Liquid Na-Pb Alloys Studied by Neutron Diffraction
N.M.Blagoveshchenskii, V.A.Morozov, A.G.Novikov, D.V.Savostin, V.V.Savostin, A.L.Shimkevich

Influence of Fe Intercalation on Phonon Density of States of $TiSe_2$
A.N.Titov, S.G.Titova, A.N.Skomorokhov, V.A.Semenov

Small-Angle Scattering

Effect of CnNO Surfactants on the DOPC Bilayer Thickness in Unilamellar Liposomes: SANS Study
D.Uhrikova, A.Islamov, A.Kuklin, F.Devinsky, I.Lacko, P.Balgavy

Small-Angle Neutron Scattering from Highly Stable Water-Based Ferrofluids
M.Balasoiu, M.V.Avdeev, V.L.Akenov, D.Bica, L.Vekas

Moleular Dynamics Simulations of Solution of Fullerene C60 in Carbon Disulfide
A.Yu.Teterev, M.V.Avdeev, M.Kholmurodov, V.L.Aksenov

4.2. NEUTRON NUCLEAR PHYSICS

Nuclear Structure

General Trend in the Changing of Nuclear Excited States Structure
V.A.Khitrov, A.M.Sukhovoj

Applied Research

Neutron for Studying Synthesis of Fine Crystalline Diamonds
M.V.Frontasyeva, S.S.Pavlov, A.G.Dutov, V.A.Komar, V.B.Shipilo, N.V.Shipilo, I.I.Azarko

NAA and AAS for Studying Elemental Content of Staple Foodstuffs in Central Russia
M.V.Frontasyeva, S.F.Gundorina, A.V.Gorbunov, S.M.Lyapunov, O.I.Okina

Epithermal Neutron Activation Analysis for Freshwater Ecosystem Monitoring: the Rybinsk Reservoir Case Study
M.V.Frontasyeva, D.F.Pavlov, S.S.Pavlov

ENAA and AAS for Analysis of Surface Soil: Example from the Thrace Region, Turkey
S.V.Demkina, M.V.Frontasyeva, Mahmut Coskin, Munevver Coskin, E.Steinnes

Use of ENAA to Study Metal Pollution in the Vicinity of Thermal Power Plants in Central Russia
E.Ermakova, M.V.Frontasyeva, E.Steinnes

COMPARATIVE STUDY OF THE MAGNETIC PHASE DIAGRAMS OF NEARLY HALF-DOPED $Sm_{1-X}Sr_XMnO_3$ WITH ^{16}O AND ^{18}O ISOTOPES

A.M. Balagurov[1)], N.A. Babushkina[2)], E.A. Chistotina[2)], I.A. Bobrikov[1)], V.Yu. Pomjakushin[3)], A.I. Kurbakov[4)], V.A. Trunov[4)], O.Yu. Gorbenko[5)], A.R. Kaul[5)], K.I. Kugel[6)]

[1)] *Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow region, 141980 Russia*
[2)] *Russian Research Center "Kurchatov Institute", Kurchatov sqr. 1, Moscow, 123182 Russia*
[3)] *Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, CH-5232, Villigen PSI, Switzerland*
[4)] *Saint Petersburg Institute of Nuclear Physics, RAS, Gatchina, Leningrad region, 188300 Russia*
[5)] *Department of Chemistry, Moscow State University, Vorobievy Gory, Moscow 119899, Russia*
[6)] *Institute for Theoretical and Applied Electrodynamics, RAS, Izhorskaya str. 13/19, Moscow, 125412 Russia*

Recent experimental and theoretical studies clearly demonstrate the importance of the existence of various-scale phase separation in the perovskite manganites $R_{1-x}A_xMnO_3$, where R is a rare earth element and A is an alkaline earth element. Both microscopic (~ 15 – 20 Å) and mesoscopic (~ 500 – 2000 Å) phase separation has been experimentally revealed and theoretically analyzed (see, for instance, Ref. [1, 2] and references therein).

The mesoscopic phase separation, which at low temperatures is often manifests itself in the form of incoherent mixture of ferromagnetic metallic and antiferromagnetic insulating domains is most clearly pronounced near the crossover between metallic and insulating states, where their ground-state energies are close to each other. A good example for such a behavior is provided by the $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ compound with y = 0.75, where, as a consequence of phase separated state, the giant oxygen isotope effect (a metal-insulator transition induced by $^{16}O \rightarrow ^{18}O$ substitution) takes place. The neutron diffraction experiments with this compound revealed that the changes in electrical transport properties correlate with the changes in magnetic structure: at the temperature lowering the sample with ^{16}O undergoes subsequent antiferromagnetic (with the CE-type ordering, T_{AFM}=145 K) and ferromagnetic (T_{FM}=115 K) transitions, resulting in incoherent mixture of ferro- and antiferromagnetic regions, while in the sample with ^{18}O the homogeneous AFM structure of CE-type (T_{AFM}=145 K) is found [3].

Extending these investigations to other systems, we studied the effect of oxygen isotope substitution on the magnetic structure of $Sm_{1-x}Sr_xMnO_3$ (SSM-x) manganites with x close to 0.5, i.e. in region where the hole doping is changing to the electron one. Such a change could also favor the phase separation. In paper [4], a pronounced oxygen isotope effect was reported for Sm-Sr compositions close to x = 0.5 and even the transition to the insulating state (at x = 0.475 and 0.5) was observed. The implementation of neutron diffraction to the study of the crystal and magnetic structure of Sm-containing manganites is quite problematic due to the very large neutron absorption in natural samarium. However, the situation can be substantially improved by using samples with the ^{152}Sm isotope for neutron experiments. The detailed diffraction experiments with $^{152}Sm_{0.55}Sr_{045}Mn^{16}O_3$, $^{152}Sm_{0.55}Sr_{045}Mn^{18}O_3$, $^{152}Sm_{0.5}Sr_{05}Mn^{16}O_3$, and

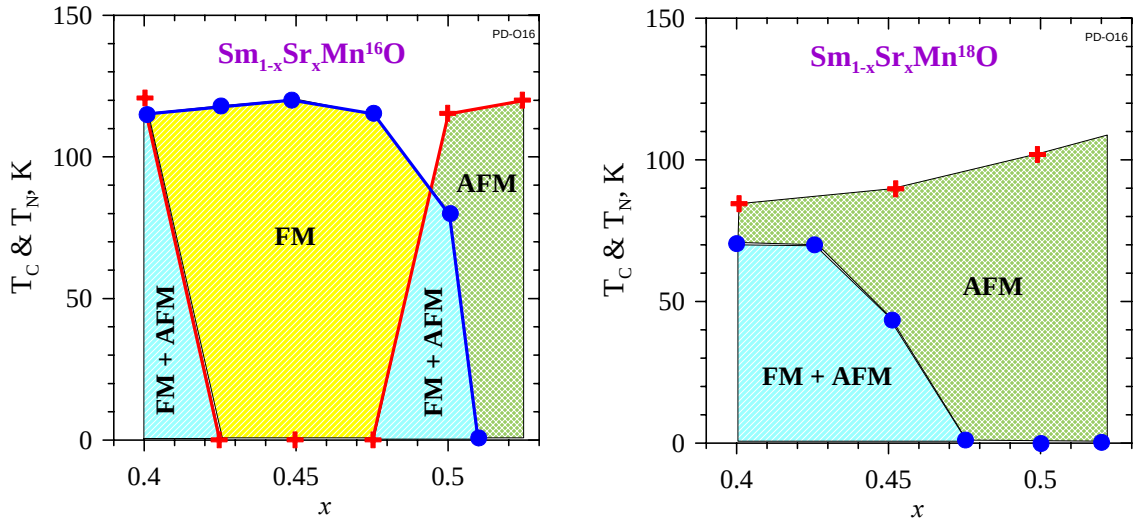

Fig. 1. Phase diagram of nearly half-doped $Sm_{1-x}Sr_xMnO_3$ manganites with ^{16}O and ^{18}O isotopes. The regions correspond to the FM, AFM and mixed FM + AFM phases are shown. For sample with ^{16}O and x=0.5 the giant isotope effect (the transformation from metallic into insulating state after $^{16}O \rightarrow {}^{18}O$ exchange) has been found.

$^{152}Sm_{0.5}Sr_{05}Mn^{18}O_3$ compositions allowed us to determine unambiguously the types of magnetic ordering and their evolution with temperature. For SSM-45-^{16}O the existence of only FM phase ($T_C \approx 120$ K, μ_{FM}=3.24 μ_B) was established, while in SSM-45-^{18}O inhomogeneous state FM + AFM_A (μ_{FM} = 0.8 μ_B, μ_{AFM} = 1.7 μ_B) was found below 100 K. Vice versa, the SSM-50-^{16}O was found in a mixed FM (μ_{FM}=2.8 μ_B) and AFM_A (μ_{AFM}=1.9 μ_B) state with dominant FM phase, whereas the ground magnetic state for SSM-50-^{18}O sample is purely A-type antiferromagnetic (μ_{AF} = 1.7 μ_B). The reduced ordered magnetic moment in SSM-50-^{18}O is an indication that the AFM phase fills only a part of the sample volume. The mean ordered magnetic moment at Mn ion in SSM-50-^{16}O ($\mu_{Mn} = (\mu^2_{FM} + \mu^2_{AFM})^{1/2}$) is equal to 3.4 μ_B. This value is very close to the expected mean value, calculated under assumption that the structure contains 50% Mn^{3+} (μ=4 μ_B) and 50% Mn^{4+} (μ=3 μ_B). Assuming that magnetic moments of Mn ions are the same both in FM and AFM phases, one can find that they occupy approximately 68% and 32% of the sample volume, respectively.

Based on the whole set of our results, we are able to draw and compare the phase diagrams of SSM-*x* with both oxygen isotopes (Fig. 1). The comparison of the changes in SSM-*x* phase diagrams due to the oxygen isotope substitution (^{16}O by ^{18}O) shows that they are first of all related to the suppression of stability for the ferromagnetic metallic state: (1) the isotope substitution is accompanied by the appreciable lowering of the Curie temperatures for all compositions; (2) a narrow region of existence for homogeneous ferromagnetic state disappears; (3) the AFM ordering is observed now for all compositions under study. The similar situation takes place for phase diagram of LPCM-*y* compound, which also exhibits a metal-insulator transition induced by oxygen isotope substitution, but with formation of AFM_{CE} state [5]. In SSM-x insulating phase close to x =0.5, we have the *A*-type AFM ordering with $d(x^2\text{-}y^2)$-type orbitals. In this sense, SSM-x differs drastically from LPCM-*y* compound. Thus, the manifestations of the isotope effect in manganites seem to be not closely related to the macroscopic features of their insulating state. The oxygen isotope substitution shifts the energy

balance between metallic and insulating state and the metal-insulator transition can be interpreted as a percolation effect independent on the magnetic structure of the insulating phase.

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CRYSTAL STRUCTURE OF LITHIUM BERYLLIUM DEUTERIDE Li_2BeD_4

B.M. Bulychev[1)], R.V. Shpanchenko[1)], E.V. Antipov[1)],
D.V. Sheptyakov[2)], S.N. Bushmeleva[3)], A.M. Balagurov[3)]

[1)] *Department of Chemistry, Moscow State University, Vorobievy Gory, Moscow 119899, Russia*
[2)] *Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, CH-5232, Villigen PSI, Switzerland*
[3)] *Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Moscow region, 141980 Russia*

Recent developments in hydrogen power engineering have resulted in a revival of interest to the chemistry of covalent and ionic complex hydrides of light non-transition metals. Special interest is being paid to the compounds with high hydrogen content, which is necessary for its extraction and further use in chemical reactions or for combustion in the fuel elements. A hydrogen capacity which determines the amount of available energy is the second critical value for proposed materials beside a cycling performance. From this point of view, the lithium beryllium hydrides are good candidates for hydrogen storage. Namely, the hydrogen capacities for $LiBeH_3$ and Li_2BeH_4 compounds are 15.9 and 15.0 wt.%, respectively. Only two known hydrides, namely BeH_2 and $LiBH_4$, have higher capacities (18.3 and 18.5, respectively). Although the lightest ternary hydrides could hypothetically be formed in the Li-Be-H system, the synthetic problems and especially difficulties in their structure characterization make this class of compounds extremely hard for investigations.

A number of attempts to index and solve the crystal structure of Li_2BeH_4 have been undertaken in the past. The first satisfactory lattice determination was presented by our group a few years ago based on X-ray powder data obtained for the Li_2BeD_4 sample placed in the sealed capillary and the $P2_1/c$ space group was proposed based on systematic extinctions [1]. However, at that time we could not find any proper crystal structure solution. The main problem of the X-ray structural analysis for the compounds with low atomic numbers is their poor scattering ability for the incident X-rays. In our case, all three elements constituting the compound are very light. This causes severe problems for the casual X-ray experiment; in particular, it requires the counting times on the order of days even for the poorest statistics. The natural way out of this complication is the use of neutron diffraction as a complementary technique with another set of scattering lengths of the elements.

X-ray powder diffraction (XPD) data were collected on automated STADI/P diffractometer ($Cu_{K\alpha 1}$-radiation, Ge monochromator, Debye-Scherrer mode, scintillation counter). Experimental data were collected during 7 days because of the low scattering properties of elements. Neutron powder diffraction (NPD) experiment was performed with a high resolution Fourier diffractometer (HRFD) at the IBR-2 pulsed reactor in Dubna with the instrumental resolution close to $\Delta d/d$=0.001. Indexing of the XPD pattern was performed with the Treor program [2]. EXPO [3] and FOX [4] programs were used for structure model construction. The refinement of the crystal structure parameters was carried out with MRIA and GSAS programs. In the latest case both XPD and NPD datasets were used simultaneously for fitting procedure.

XPD pattern of Li_2BeD_4 was indexed in monoclinic cell with lattice parameters

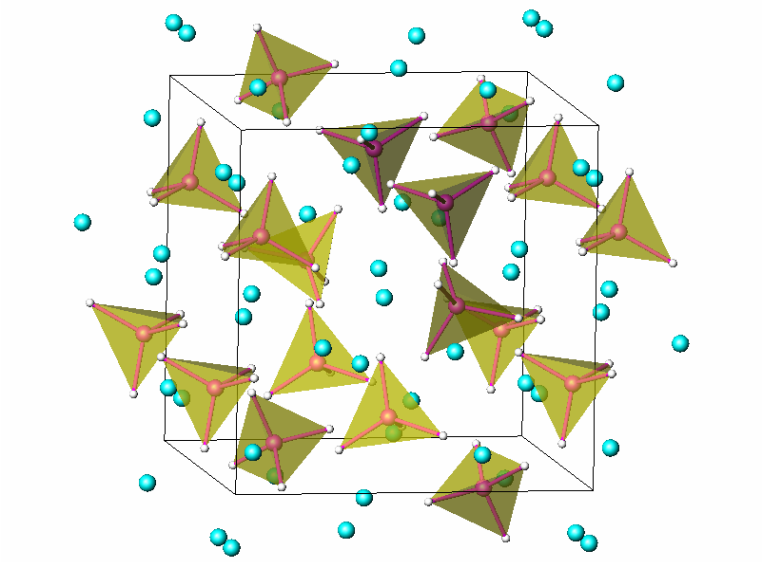

Fig.1. Crystal structure of Li_2BeD_4 as revealed by neutron diffraction.

a = 7.0969(9) Å, b = 8.374(2) Å, c = 8.384(2) Å, β = 93.69(1)°, V = 490.37(1), Z = 8. No visible admixture peaks were observed. Since the only $h0l$: l=2n and $0k0$: k=2n extinction conditions could be deduced from the peak list obtained by pattern fitting the $P2_1/c$ space group was chosen for structure solution. The correctness of the found indexing solution is confirmed also by good agreement of the calculated 0.72 g/cm^3 and measured 0.71 g/cm^3 (for Li_2BeH_4) densities. One should note that X-ray patterns of Li_2BeD_4 and Li_2BeH_4 are almost identical and lattice parameters remained unchanged regardless of starting composition and phases present. Although the X-ray pattern of Li_2BeD_4 was successfully indexed, we failed to find the crystal structure solution using only the XRD data. The direct methods implemented in the EXPO program complex in application to the neutron diffraction dataset were utilized at the beginning of the structure solution process. The attempt to locate the lithium atoms by direct methods with the neutron diffraction dataset was, however, unsuccessful – due to the relatively weak scattering ability of lithium atoms for neutrons. On the other hand, Li atoms are in a comparatively better contrast in the X-ray diffraction case, especially if the BeH_4 tetrahedra are already located in the structure. The next step therefore, was the using of the ab-initio global optimization algorithm implemented in the FOX program and applied to the X-ray dataset. The BeD_4 tetrahedra found in the first step were incorporated in the Li_2BeD_4 unit cell and their position and orientations were fixed. After that, the positions of four lithium atoms were found starting from the completely random configuration.

The Rietveld refinement of the Li_2BeD_4 crystal structure was carried out simultaneously for the XPD and the room temperature NPD (TOF) datasets. Thermal parameters were constrained to equality within the different atom types. The compound has monoclinic unit cell (S.G. $P2_1/c$) with lattice parameters a = 7.06228(9) Å, b = 8.3378(1) Å, c = 8.3465(1) Å, β =93.577(1)°, Z = 8. Its structure contains isolated BeD_4 tetrahedra, and Li atoms are located in the structure interstices (Fig.1). Li_2BeD_4 does not undergo any structural phase transitions down to 8 K.

The crystal structure determination of Li_2BeD_4 is the first reliable result of structure solution for the ternary hydride in the Li-Be-H system. This example demonstrates the power of modern software for the direct structure determinations from powder diffraction data and the

advantages of the simultaneous use of neutron and X-ray diffraction data for structural characterization of compounds in the lightest ternary system even the quality of diffraction data is not very high.

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PRESSURE INDUCED PHASE TRANSITION IN FERROELECTRIC PIRYDINIUM PERRHENATE

P. Czarnecki[a], A. I. Beskrovny[b], L. Bobrowicz-Sarga[a], S. Lewicki[a] and J. Wąsicki[a]

[a]*Faculty of Physics, A. Mickiewicz University, ul. Umultowska 85,PL- 61-614 Poznań, Poland*
[b]*Frank Laboratory of Neutron Physics, JINR, RU-141980, Dubna, Russia*

We report results of the high pressure study of pyridinium perrhenate $PyHReO_4$ by dielectric spectroscopy, NMR and neutron diffraction. The structure of this compound [1] differs from those of the other pyridinium salts such as $PyHBF_4$ [2] and $PyHClO_4$ [3], and thus the perrhenate undergoes two phase transitions a continuous one at 336 K and a discontinuous one at 250 K. In all phases $PyHReO_4$ has orthorhombic structure and undergoes the following phase transitions: $Cmcm \rightarrow Cmc2_1 \rightarrow$ Pbca. The intermediate phase is ferroelectric, while the disordered high-temperature phase and ordered low-temperature phase are centrosymmetric. The aim of the study is to determine the p-T phase diagram and its comparison with analogous ones obtained for the rhombohedral pyridinium salts.

The high-pressure dielectric and NMR measurements were performed in a beryllium-copper high pressure cell connected with a gas compressor GCA-10 (UNIPRESS) and U11 (UNIPRESS) respectively. Neutron powder diffraction spectra (NPD) were measured by the time of flight method on a NERA-PR spectrometer working in inverted geometry. The high pressure gaseous helium set-up consists of a gas compressor U11, a Gas Neutron Cell GNC-400 and a cryostat.

Systematic dielectric and NMR measurements performed at a few pressures and in a temperature range from 154 K to 300 K permitted drawing the p-T diagram presented in figure 1. At about 100 MPa and at 240 K there is a triple point joining two curves of phase equilibrium. In order to verify the presence of the pressure-induced phase we have performed neutron diffraction measurements under varying pressure.

At 230 K neutron diffraction spectra were measured at a few pressure values (Fig. 2): 0.1 MPa, 80 MPa, 200 MPa, 370 MPa and at 260K at 370 MPa. The neutron diffraction spectra recorded at 230 K and at the pressures 200 MPa and 370 MPa differ from those recorded at 80 MPa and 0.1 MPa, which proves the presence of a new pressure-induced phase. The change in the diffraction spectrum recorded at 370 MPa when changing the temperature of measurement from 230 K to 260 K also confirms the presence of a new phase transition between the pressure-induced phase II` and phase II. The volume expansion coefficients α as well as the compressibility β have been determined.

The p-T phase diagram obtained for $PyHReO_4$ differs significantly from those of the other pyridinium ferroelectric salts $PyHBF_4$ [4], $PyHClO_4$ [5]. In $PyHReO_4$ the temperatures of both phase transitions are shifted towards lower values with increasing pressure, whereas for $PyHBF_4$ and $PyHClO_4$ they are shifted towards higher values. The pressure dependence of the continuous phase transition temperature (T_1) follows the Ehrenfest equation

The phase transition at T_2 is discontinuous. The pressure dependence of discontinuous phase transitions is described by the Claussius-Clapeyron equation:

The shift of T_2 towards lower values under the effect of elevated pressure in $PyHReO_4$ is caused by a small negative jump change in volume $\Delta V \approx -3$ [$Å^3$] at T_2=250K.

The symmetry of the pressure-induced phase II` could not be determined from the NPD measurements, however, the character of the temperature dependencies obtained in the NMR experiment suggest that this phase is partly disordered and thus similar to phase III.

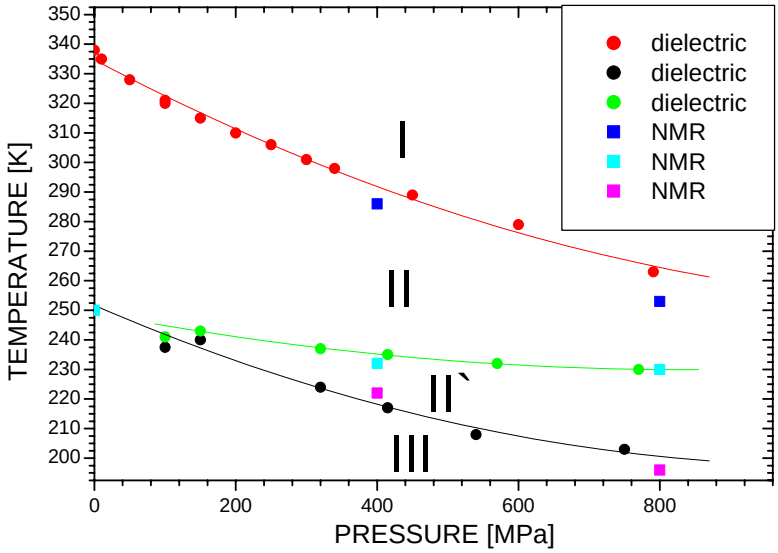

Fig.1. p-T phase diagram of $PyHReO_4$.

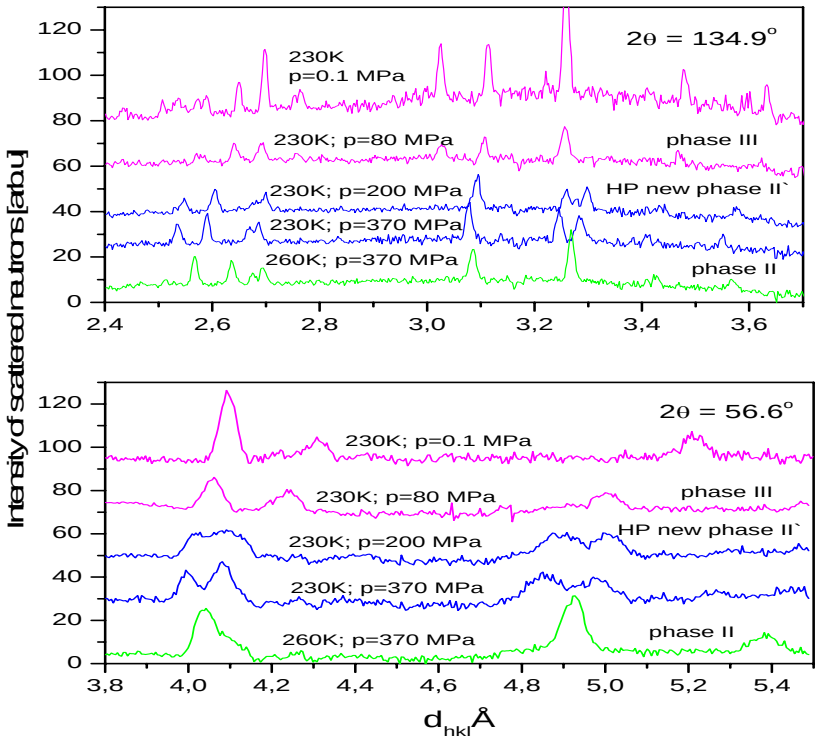

Fig.2. Neutron powder diffraction spectra measured at a few pressures.

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TEMPERATURE- AND COMPOSITION-DRIVEN CHANGES OF MAGNETIC MOMENTS AND LATTICE PARAMETERS IN QUASIBINARY $(Sc_{1-x}Y_x)Fe_2$ LAVES PHASE COMPOUNDS

Z. Surowiec[a)], A. I. Beskrovnyi[b)], M. Wiertel [a)], J. Sarzyński [a)], M. Budzyński [a)]

[a)] *Institute of Physics, UMCS, pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland*
[b)] *Frank Laboratory of Neutron Physics, JINR 141980 Dubna, Moscow Reg., Russia*

The experimental investigations of quasibinary alloys such as $(A_{1-x}A'_x)B_2$ are interesting for two main reasons. On the one hand it's the searching of materials with the determined magnetic, electrical and mechanical properties, on the other, it's the creation of the experimental basis for the theoretical study of the itinerant electron magnetism.

The compounds under discussion formed the quasibinary Laves phases in which Y atoms replaced a part of Sc atoms. Such a replacement is strongly suggested both by atomic sizes of the Y and Sc atoms (respectively 1.80 and 1.60 Å) and their chemical similarity (Pauling electronegativities: 1.22 and 1.36 respectively).

In the quasibinary system of $ScFe_2$ and YFe_2 Laves phases the crystal structure changes from the hexagonal C14 type ($MgZn_2$, space group $P6_3/mmc$) to the cubic C15 type ($MgCu_2$, space group $Fd3m$). In the cubic phase Fe atoms create regular tetrahedrons (*16d* positions of the $\bar{3}m$ point symmetry) connected via their corners. In the hexagonal phase Fe atoms form the sublattice of regular tetrahedra linked alternately by their apexes (*2a* positions of the $\bar{3}m$ point symmetry) or by their bases (*6h* positions of the *mm* point symmetry). The A or A' atoms occupy *8a* crystallographic sites ($\bar{4}3m$ point symmetry) in C15-type structure and *4f* sites (*3m* point symmetry) in C14-type structure. In the both structures the nearest neighbour of Fe atoms is composed of six Fe and six Sc(Y) atoms. The $ScFe_2$ and YFe_2 compounds are ferromagnetism with an almost the same $T_C \approx 542$ K [1].The measurements [2, 3] and the electronic structure calculations [4, 5] for these compounds gave the Fe magnetic moments values of about 1.5 μ_B and an antiparallel moments of about -0.6 μ_B induced at Sc and Y sites as a result of the hybridization of *3d* Fe and *3d* Sc or 4d Y bands. The [001] direction in $ScFe_2$ and [111] in YFe_2 are the magnetic moments ordering axes.

The quasibinary $(Sc_{1-x}Y_x)Fe_2$ compounds were prepared by arc melting appropriate stoichiometric quantities of Sc, Y and Fe of high purity (no lower than 4N), in an inertial argon atmosphere. The structure of samples was examined by XRD measurements. The single cubic C15 phase was found in the samples with x=0.20 and 0.50 and the main hexagonal C14 phase in the $ScFe_2$. Only a few weak peaks of an unidentified foreign were detected in this sample.

The neutron diffraction (ND) experiments were performed with the DN2 time-of-flight powder diffractometer at the fast pulsed reactor, IBR-2 in the Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research. The diffraction patterns were refined by the FULLPROF Rietveld refinement program. A convolution pseudo-Voigt with double exponential function was chosen to generate the line shape of the diffraction peaks. In the final run the following parameters were refined from the ND data: scale factor, background coefficients, unit-cell parameters, pseudo-Voigt parameter, positional coordinates, isotropic thermal factors and the magnitude of the Fe and Sc(Y) ordered magnetic moments. The coherent scattering lengths for Fe, Sc and Y were taken as 9.45, 12.29 and 7.75 *fm,* respectively. At temperatures below T_C the fittings are performed assuming the magnetic ordering models described in [2−5].

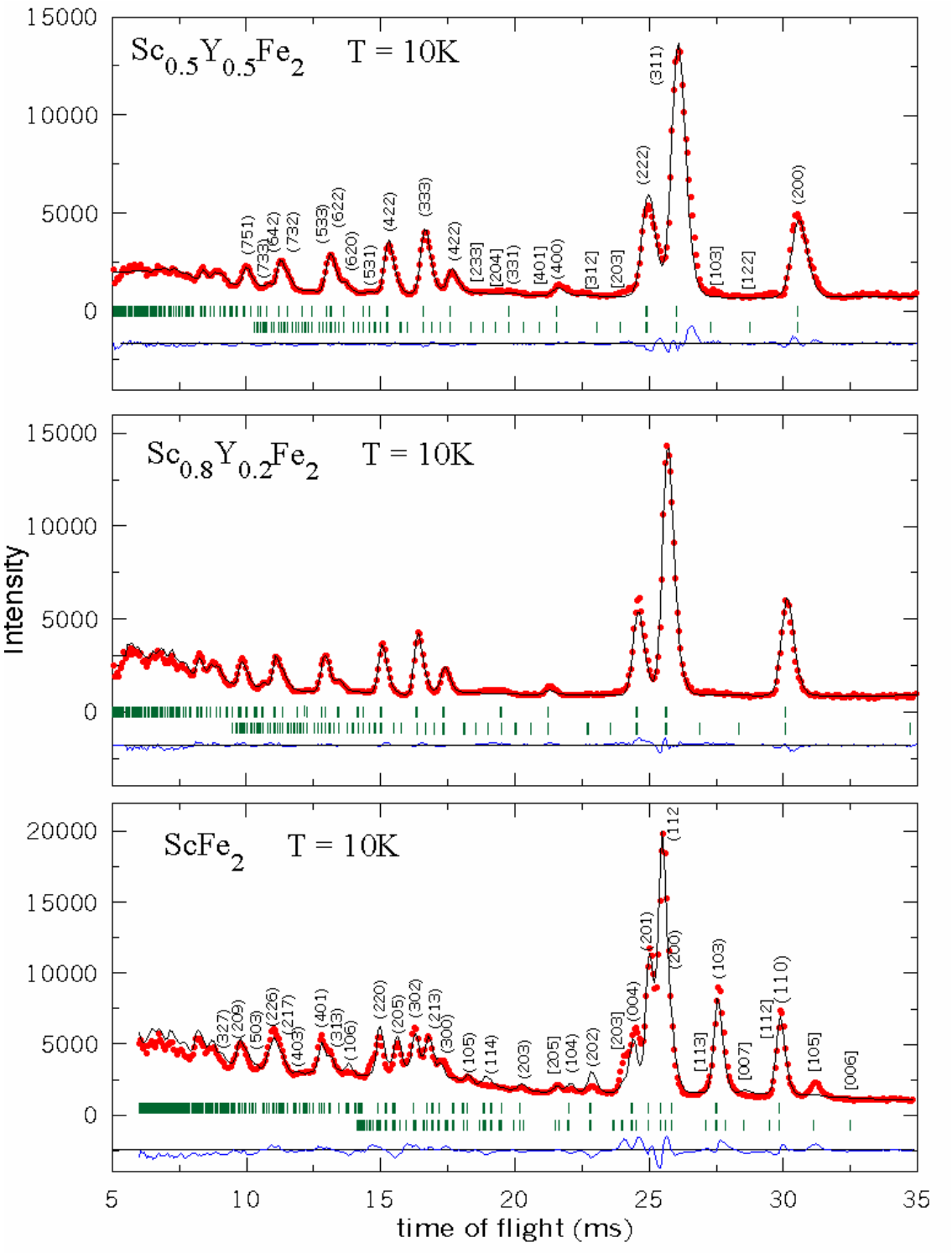

Fig. 1. The time-of-flight spectra measured by means of the DN2 diffractometer at 10 K for $(Sc_{1-x}Y_x)Fe_2$ compounds with x =0.0, 0.2 and 0.5, respectively. The full lines represent the calculated pattern, the points the observed one and the lower curves the difference between observations and calculations. Short vertical marks below the diffraction pattern indicate the calculated nuclear Bragg positions (upper row) and the magnetic ones (lower row).

Neutron diffraction measurements were made as a function of temperature between 10 K and 620 K for $(Sc_{1-x}Y_x)Fe_2$ samples with $x \leq 0.5$. Figure 1 shows a section of the time-of-flight powder diffraction spectra for the investigated compounds with x = 0.0, 0.2 and 0.5, respectively, measured at 10 K.

A good agreement between the experimental and calculated spectra is obtained for the quasibinary samples with reliability factor R less then 5 %. The poor fitted peak overlapping with the magnetic (105) peak in the $ScFe_2$ compound is observed also above T_C and belongs to an unidentified foreign phase.

Table 1. Magnetic moments of Fe atoms, the mean magnetic moments induced at Y and Sc sites by the Fe sublattice in the intermetallic $Sc_{1-x}Y_xFe_2$ compounds and the distance between Fe atoms in nearest neighbour for the different Y concentrations x and temperatures.

x	T [K]	μ_{Fe} [μ_B]	$\mu_{Sc/Y}$ [μ_B]	d_{Fe-Fe} [Å]
0.5	10	1,69(8)	-0,66(8)	2,524(5)
	300	1,22(9)	-0,47(10)	2,533(5)
0.2	10	1,43(8)	-0,63(8)	2.498(5)
	300	1,08(9)	-0,45(9)	2,507(5)
0.0	10	1,24(10)	-0,58(8)	2,460(5)
	300	0,85(10)	-0,40(9)	2,480(5)

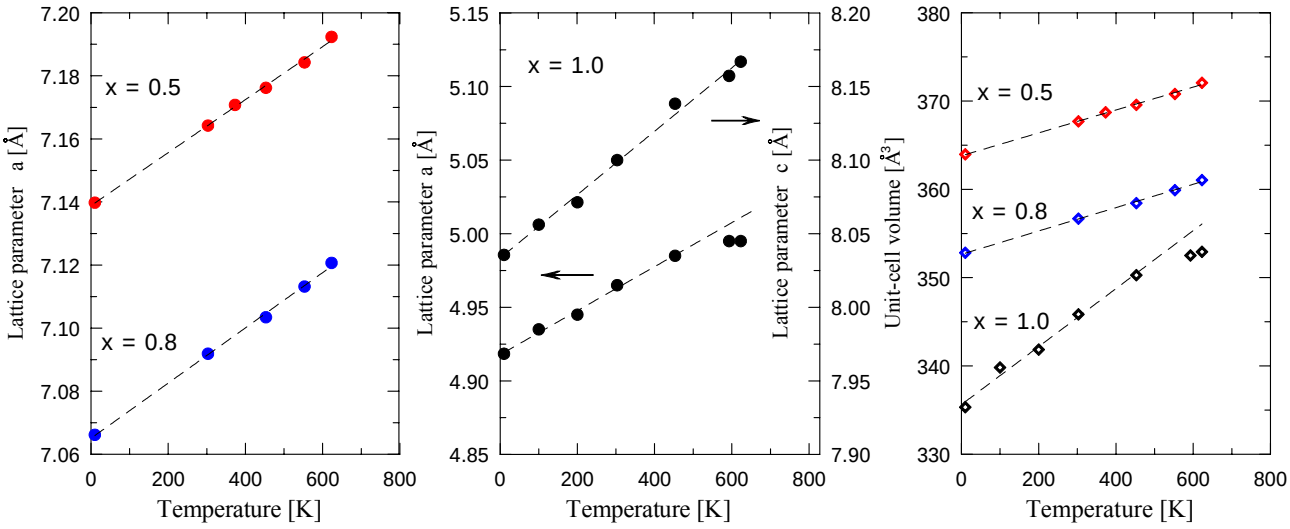

Fig. 2. The temperature dependencies deduced from powder ND data for lattice parameters and unit-cell volume in $(Sc_{1-x}Y_x)Fe_2$ compounds with x =0.5, 0.8 and 0.0, respectively.

The magnetic moments and distances between Fe atoms in the nearest neighbour obtained from the refinements are given in Table 1. The results for $ScFe_2$ remain in the qualitative accordance with values available in literature [2,6] and with the results of theoretical calculations [4]. The replacement of Sc atoms by Y atoms leads to the structural C14 → C15 transformation and simultaneously yields a decrease in the magnetic moments. The strong dependence these moments on the Fe−Fe distance is characteristic for the discussed materials in which the itinerant electron magnetism is responsible for magnetic properties. The reduction of Fe magnetic moments with decreasing the Fe−Fe distance was observed also in $(Sc_{1-x}Ti_x)Fe_2$ where the lattice contraction was caused by high pressure [7].

The thermal variation of the lattice parameters and the unit-cell volumes for different Y concentration *x* obtained from the neutron diffraction measurements is shown in Fig. 2. From these dependencies thermal expansion coefficients could be determined. For the samples with the cubic C15 structure $\alpha(x = 0.2) = 8{,}8(2)\cdot10^{-5}$Å/K and $\alpha(x = 0.5) = 8{,}4(2)\cdot10^{-5}$Å/K, respectively. In the case of $ScFe_2$ with hexagonal C14 structure anisotropic expansion is observed. Along the crystallographic *c* axis $\alpha_{//}(x =0) = 2{,}1(3)\cdot10^{-4}$Å/K and in the perpendicular to the [001] direction $\alpha_{\perp}(x = 1{,}0)$ $1{,}3\cdot10^{-4}$Å/K. The change of slope in the *a(T)* dependence observed at temperatures above T_C for this sample is related to a magnetostriction effect. Generally, the anharmonic component in lattice vibration clearly decreases along with the transition from the hexagonal to the cubic structure in spite of the increasing spatial disorder in the quasibinary phases.

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NEUTRON STUDY OF $MN_3FE_4V_6O_{24}$

N.Guskos[1,2], A.Beskrovnyy[3], J.Typek[2], N.Yu.Ryabova[3],
A.Blonska-Tabero[4], M.Kurzawa[4], and M.Maryniak[2]

[1]*Solid State Physics, Department of Physics, University of Athens, Panepistimiopolis, 15 784 Zografos, Athens, Greece*
[2]*Institute of Physics, Technical University of Szczecin, Al.Piastow 17, 70-310 Szczecin, Poland*
[3]*Frank Laboratory of Neutron Physics, Join Institute for Nuclear Research, 141980 Dubna, Russia*
[4]*Department of Inorganic and Analytical Chemistry, Technical University of Szczecin, Al.Piastow 17, 70-310 Szczecin, Poland*

Polycrystalline samples of $Mn_3Fe_4V_6O_{24}$ were obtained from a solid-state reaction between MnO, V_2O_5 and Fe_2O_3 mixed at a molar ratio 3:2:2, according to the equation [1]:

$$3MnO + 3V_2O_5 + 2Fe_2O_3 = Mn_3Fe_4V_6O_{24}$$

The crystal structure of the $Mn_3Fe_4V_6O_{24}$ compound was investigated by the neutron powder diffraction method by using a high luminosity DN-2 time-of-flight powder diffractometer at the IBR-2 pulsed reactor at the FLNF Frank Laboratory of the Joint Institute of Nuclear Research (JINR), Dubna in Russia. The neutron diffraction patterns were measured with resolution determined by the width of the pulse from a neutron source, $\Delta d/d=0.01$ in the range of interplanar spacings d_{hkl} from 1 to 20 Å. The diffraction patterns were collected employing approximately 10 g of the sample, enclosed in a thin-walled aluminium cylindrical container of 8 mm in diameter. The counting time was 15 h for every point at a specific temperature. The diffraction patterns were obtained at temperatures of 10 K and 290 K and analyzed by the program MRIA (Multi-phase Rietveld Analysis) [2] using X-ray diffraction data for β-$Cu_3Fe_4V_6O_{24}$ as a starting model for Rietveld refinement [3].

Neutron diffraction spectra of different profiles obtained at 10 K and 290 K for $Mn_3Fe_4V_6O_{24}$ compound are presented in Figure 1. The diffraction pattern did not show any magnetic contribution at investigated temperatures for the $Mn_3Fe_4V_6O_{24}$ compound. Figure 2 presents neutron diffraction spectrum of $Mn_3Fe_4V_6O_{24}$ and the simulated spectrum calculated by the program MRIA (χ^2=1.70). As could be seen a good agreement was obtained between the experimental and the calculated spectrum.

$Mn_3Fe_4V_6O_{24}$ crystallizes in the triclinic system. The parameters of the unit cell determined from neutron diffraction (at both temperatures: 10K and 290K) and XRD analysis are presented in Table 1.

The value of unit cell parameters increase with the increasing temperature and some discrepancy is observed between the neutron diffraction and XRD data (Table 1). The bulk crystal unit parameters have been changed by the temperature change in the following way: $\Delta a_T = 0.003$Å, $\Delta b_T = 0.008$Å, $\Delta c_T = 0.012$Å, and the volume change $\Delta V_T = 1.5$Å^3. As it could seen the thermal expansion processes is strongly anisotropic being the largest in the **c** direction and weakest in the **a** direction.

$Mn_3Fe_4V_6O_{24}$ compound is a homeotype of β-$Cu_3Fe_4V_6O_{24}$ since the structure is build up from $M(1)O_6$ polyhedra, $M(2)O_5$ trigonal bipyramids, $M(3)O_6$ and $M(4)O_6$ octahedra and isolated VO_4 tetrahedra. Fe_2O_{10} octahedral dimers alternate with $M(2)O_5$ bipyramids to form

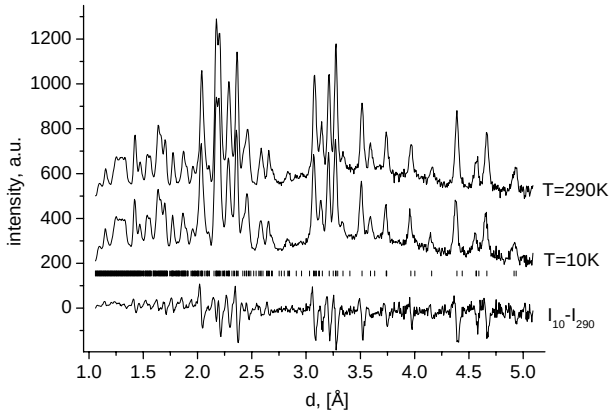

Fig.1. Neutron diffraction spectra of $Mn_3Fe_4V_6O_{24}$ obtained in the range of d_{hkl} up to 11 at temperatures 10K and 290K.

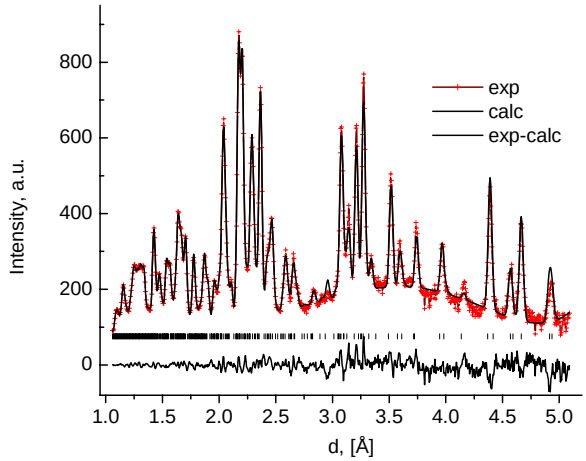

Fig.2. Neutron diffraction spectrum of $Mn_3Fe_4V_6O_{24}$ and simulated spectrum obtained by MRIA program (χ^2=1.70) at temperature 290K.

edge-sharing chains (Fe(1) and Fe(2) are in position M(3) and M(4), respectively). The $M(1)O_6$ octahedra are located between the chains and share corners with both the $M(2)O_5$ and Fe_2O_{10} units. Figure 3 presents the projection of the structure along [100] axis.
The neutron diffraction study of powder of $Mn_3Fe_4V_6O_{24}$ has shown that the iron(III) and manganese(II) ions are disordered in structure, and the distribution on the octahedral and the trigonal bipyramidal sites are non-statistical:

M(1) = Mn; M(2) = 1.60(2) Mn+0.40(2) Fe;
M(3) = 0.08(2) Mn+1.92(2) Fe; M(4) = 0.32(2) Mn+1.68(2) Fe.

The temperature dependence of the metal-oxygen lengths for $Mn_3Fe_4V_6O_{24}$ could be calculated from the 290 K and 10 K measurements and the following values are obtained:

Δd_{1T}=<M(1)-O>$_{[4+2]}$(290) − <M(1)-O>$_{[4+2]}$(10) = 0.009Å;
Δd_{2T}=<M(1)-O>$_{[4]}$(290) − <M(1)-O>$_{[4]}$(10) = 0.002Å;
Δd_{3T}= <M(2)-O>$_{[5]}$(290) − <M(2)-O>$_{[5]}$(10) = − 0.052Å;
Δd_{4T}=<M(3)-O>$_{[6]}$(290) − <M(3)-O>$_{[6]}$(10) = − 0.004Å и
Δd_{5T}=<M(4)-O>$_{[6]}$(290) − <M(4)-O>$_{[6]}$(10) = 0.003Å.

The thermal expansion processes is dominated by changes in distances involving M(2) position. Down to the temperature of 10 K no magnetic long-range order has been observed.

Table 1. Crystallographic data for $Mn_3Fe_4V_6O_{24}$ obtained from the neutron diffraction (at 10K and 290K) and XRD at room temperature.

Parameter	T=290K	T=10K	X-ray [1]
fw	1077.84		
Space group	*P*-1 (no.2)		
a [Å]	6.7041(5)	6.7014(5)	6.703(2)
b [Å]	8.1487(7)	8.1410(7)	8.137(1)
c [Å]	9.8121(7)	9.8006(7)	9.801(2)
α [°]	105.51(1)	105.47(1)	105.56(1)
β [°]	105.54(1)	105.66(1)	105.58(2)
γ [°]	102.37(1)	102.41(1)	102.35(1)
V [Å^3]	473.4(1)	471.9(1)	471.9(2)
Z	1		
d_{calc} [g/cm^3]	3.78	3.78	3.79
R_p	2.96	2.78	-
R_w	1.94	1.60	-
χ^2	1.70	1.60	-

$\chi^2=\sum w(I_e - I_c)^2$; $R_w=[\sum w(I_e - I_c)^2/\sum wI_e^2]^{1/2}$; $R_p=\sum| I_e - I_c |/\sum| I_e |$.

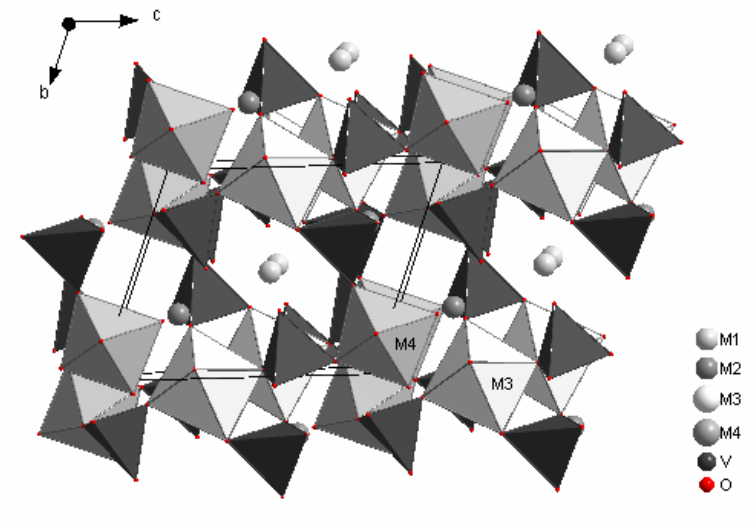

Fig.3. Crystal structure of $Mn_3Fe_4V_6O_{24}$ viewed along the a-axis.

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HIGH PRESSURE EFFECTS ON THE CRYSTAL AND MAGNETIC STRUCTURE OF $PR_{1-X}SR_XMNO_3$ MANGANITES (X = 0.48, 0.85)

D. P. Kozlenko[1], V. P. Glazkov[2], Z. Jirák[3], B. N. Savenko[1] and S.E.Kichanov[1]

[1] *Frank Laboratory of Neutron Physics, JINR, 141980 Dubna Moscow Reg., Russia*
[2] *Russian Research Center "Kurchatov Institute", 123182 Moscow, Russia*
[3] *Institute of Physics, Cukrovarnická 10, 162 53 Prague 6, Czech Republic*

Manganites of perovskite type $A_{1-x}A'_xMnO_3$ (A - rare earth, A' - alkali earth elements) exhibit rich magnetic and electronic phase diagrams depending on the A (A') - site elements and show an extreme sensitivity of magnetic, structural, electronic and transport properties to variation of temperature, external high pressures and magnetic fields. These systems have attracted considerable interest with respect to the recently discovered colossal magnetoresistance (CMR) effect. The properties of manganites depend substantially on a balance between the ferromagnetic (FM) interactions mediated by itinerant charge carriers (double - exchange mechanism) and the superexchange interactions between localized spins of manganese ions, which are usually antiferromagnetic (AFM) [1]. This balance can be effectively modified by the application of high external pressure leading to the change of the magnetic ground state in manganites.

The crystal and magnetic structures of the manganites $Pr_{1-x}Sr_xMnO_3$ (x = 0.48, 0.85) have been studied by means of powder neutron diffraction at high external pressures up to 4.1 GPa at the DN-12 diffractometer. At ambient pressure, both compounds have a tetragonal structure (sp. gr. *I4/mcm*). $Pr_{0.52}Sr_{0.48}MnO_3$ exhibits a ferromagnetic state below $T_C \approx 290$ K [2]. $Pr_{0.15}Sr_{0.85}MnO_3$ transforms to the C-type AFM state at $T_N \approx 260$ K [3]. At high pressure, in $Pr_{0.52}Sr_{0.48}MnO_3$ a onset of the A-type AFM state ($T_N \approx 250$ K) with a propagation vector q = (1 0 0) accompanied by the structural phase transformation from the tetragonal to the orthorhombic structure with *Fmmm* symmetry was observed (fig. 1). In the orthorhombic high pressure phase of $Pr_{0.52}Sr_{0.48}MnO_3$ MnO_6 octahedra are apically compressed along the a-axis. In $Pr_{0.15}Sr_{0.85}MnO_3$ the initial C-type AFM state remains stable over the studied pressure range 0 – 4.1 GPa.

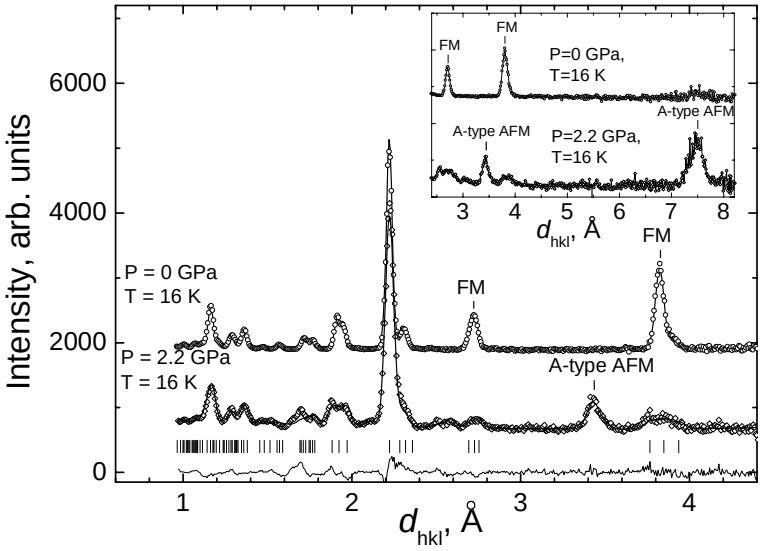

Fig. 1. *Neutron diffraction patterns of $Pr_{0.52}Sr_{0.48}MnO_3$ measured at P = 0 and 2.2 GPa, T = 16 K at scattering angles 2θ = 90° and 45.5° (inset) and processed by the Rietveld method. The appearance of the A-type AFM state with the orthorhombic structure under high pressure was observed. Ticks below correspond to the calculated positions of nuclear peaks of the orthorhombic high pressure phase.*

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IINS AND NMR STUDY OF 11 KETO PROGESTERONE

K. Hołderna-Natkaniec[1], I. Natkaniec[2,3] ,A. Szyczewski[1]

[1]*Department of Physics, A. Mickiewicz University, 61-614 Poznań, Poland.*
[2]*Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia.*
[3]*H. Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences , 31-342 Kraków, Poland.*

Steroids are low-molecular weight compounds derived from cholesterol, that play a number of important physiological roles. The subject of this study is 11-keto-progesterone (keto-prg), the corticosteroid controlling the metabolism of minerals in the organisms. Taking into regard the biological activity of the compounds and certain structural properties (cyclic compounds whose basis nucleus consists of three 6-membered rings and 5-membered cyclopentane ring, substituted at positions 10, 13, 20 by methyl groups denoted as: $C(18)H_3$, $C(19)H_3$ and $C(21)H_3$ these compounds are attractive research materials. The molecule geometry, frequency and intensity of the IINS and IR vibrational bands of keto-prg have been obtained by the HF, PM3 and density functional theory (DFT) with the B3LYP functionals and 6-31G(*d,p*) basis set. The optimised bond lengths and bond angles of the steroid skeleton are in good agreement with the X-ray data.

The IINS spectra were converted in one phonon scattering approximation to the phonon density of state function versus energy transfer (Fig.2). For hydrogenous substances, G(ν) functions represent the vibrational density of state weighted on the amplitudes of hydrogen atoms vibrations in given modes $\sim G_H(\nu)$, because the value of cross-section for incoherent neutron scattering of protons is 80.26 barns, while for carbons and oxygen is around 5.55 and 4.23 barns. The resolution power of NERA spectrometer is close to 3% in the energy transfer range below 800 cm^{-1}, then decreases to 5% when the energy transfer increases up to 1500 cm^{-1}.

The phonon density of state spectra of keto-prg recorded at 20 K was presented in Fig.2 in comparison with the *ab initio*, density functional and semiempirical methods. According to the interpretation of the IR and IINS spectra based on the quantum chemistry calculations the strong bands in the experimental G(ν) spectrum of keto-prg recorded at 20K should appear in the range 80 - 250 cm^{-1}. The G(ν) spectra of keto-prg may be compared with the spectra of progesterone, where the torsion out-of-plane bands appear nearly in the same region of energy transfer. The band corresponding to the torsional vibrations of $CC(21)H_3$ should occur at 89, 97 and 110 cm^{-1} in the spectrum of progesterone (prg) and at 111, 136, 141, 150 cm^{-1} in that of keto-prg. The torsional vibrations of the methyl group $CC(19)H_3$ should be at 220 , 252 cm^{-1} in the spectrum of prg and at 203, 221, 239 cm^{-1} in that of keto- prg (taking into account PED>10%), while for the group $CC(18)H_3$ the vibrations positions are at 141, 190, 220 cm^{-1} in the spectrum of prg and at 203, 221, 239 cm^{-1} in that

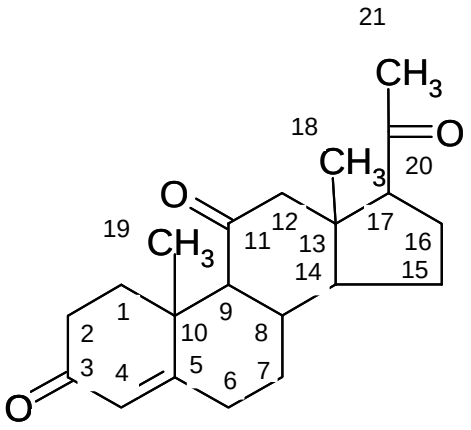

Fig.1. 4-pregnen-3,11,20-trione or 11-keto-progesterone

of keto- prg. In the spectra of both prg and keto-prg the out-of-plane torsional modes $CC(21)H_3$ are in the range of the lattice vibrations.

The harmonic vibrational wavenumbers of normal modes computed by different QC methods and corresponding experimental values are collected in fig.3. These figure presents experimental and DFT calculated values of wavenumbers. The calculated scaling coefficient SF=0.997 indicates a small effect of anharmonicity, what means that the DFT calculated vibrational wavenumbers are close to the experimental results, similar as in previous steroids studied.

Analysis of the temperature dependence of the spin-lattice relaxation times provides information on molecular dynamics of the compounds studied. The temperature dependencies of the proton spin-lattice relaxation time of 11-ketoprogesterone was interpreted using the dipolar theory first described by Bloembergen et.al. and extended by Kubo and Tomita to more than one relaxation process:

$$\left(\frac{1}{T_1}\right) = \sum_i C\left(\frac{\tau_c}{1+\omega^2\tau_{ci}{}^2} + \frac{4\tau_c}{1+4\omega^2\tau_{ci}{}^2}\right)$$

assuming that the correlation time follows an Arrhenius activation law: $\tau_{ci}=\tau_{0i}\exp[E_{ai}/RT]$. Hence we obtained possibility to estimated value of the activation parameters as: $\tau_{o1}{}' = 2*10^{-13}$ s, E'_{a1}=9.6 kJ/mol and $\tau_{o2}{}'' = 7*10^{-13}$s, E_{a2}"=12.5 kJ/mol.

In order to suggest the sequence of onset of the methyl group reorientations, the calculation of the energy of an isolated molecule versus the angle of subsequent methyl group orientation was performed by the semi-empirical PM3 method. From the dependencies of $E(\varphi)$ the heights of the barriers of the subsequent methyl groups reorientations can be obtained, in the isolated molecule approximation, as $E_a(C(18)H_3)$ = 10.2 kJ/mol, $E_a(C(19)H_3)$ = 6.0 kJ/mol and $E_a(C(21)H_3)$= 1.4 kJ/mol, respectively. Hence, the activation energy values of the reorientations of the two methyl groups $C(18)H_3$ and $C(19)H_3$ about the three-fold symmetry axis of C-C H_3 bond obtained from the spin-lattice relaxation time are close to the values 9.6 kJ/mol and 12.5 kJ/mol.

In Table 1 are collected of values of the energy transfer for torsional out-of-plane modes of subsequent methyl groups as well as the high of the barrier if internal rotation about the three-fold symmetry axis of methyl group not only in keto-prg but also in prg. The activation energies of methyl groups reorientation determined for these compounds means on different internal dynamics.

The introduction of the keto-group into the progesterone skeleton is reflected by higher value of the thermal expansion coefficient of keto-prg than prg. Moreover, the INS spectra of keto-prg at RT are smeared while those of prg are well separated and the intensity of elastic peak of keto-prg is lower than in prg. This observation can support thesis on greater mobility of protons in keto-prg at RT.

Analysis of the internal structure of 11-keto progesterone, i.e. the 11-keto substituent induces changes in the electron configuration of the C(11) atom from sp^3 to sp^2, and thus conformational changes in the neighbouring rings may take place. Also the intermolecular hydrogen bond C(12)-H(12)…O(11) and close intermolecular distance O(11) O(11) in the crystal structure of keto-prg is observed. All the structural properties could influence the thermodynamical properties, the internal dynamics of the methyl groups and in particular seem to be the reason for different behaviour of rings A and D of the steroid skeleton in keto-progesterone relative to that in progesterone, at room temperature. The internal libration of rings A and D from the carbon skeleton of 11 keto-progesterone affects the NMR spectra of keto-progesterone above 130K, while the NMR spectra of progesterone above 320K.

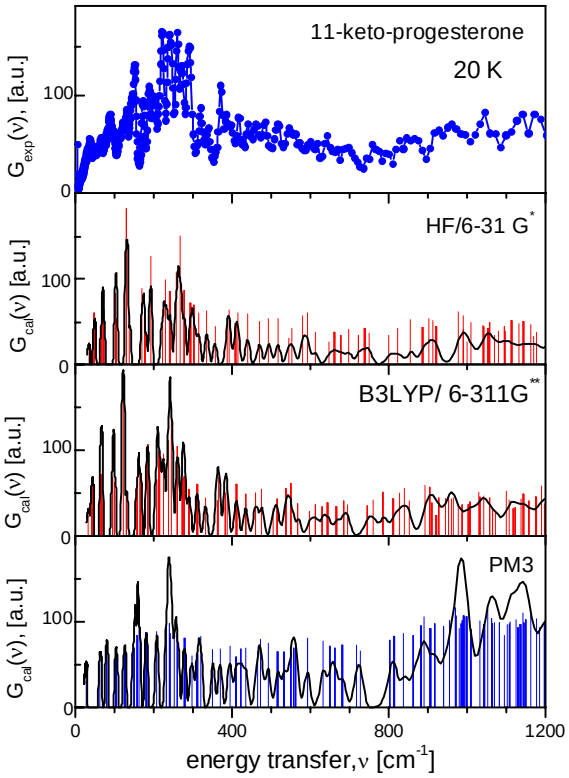

*Fig.2. Phonon density of state spectra of 11-keto progesterone obtained at 20 K compared with calculated ones by ab initio HF/6-31, density functional B3LYP/6-311 G**, and semiempirical PM3 methods.*

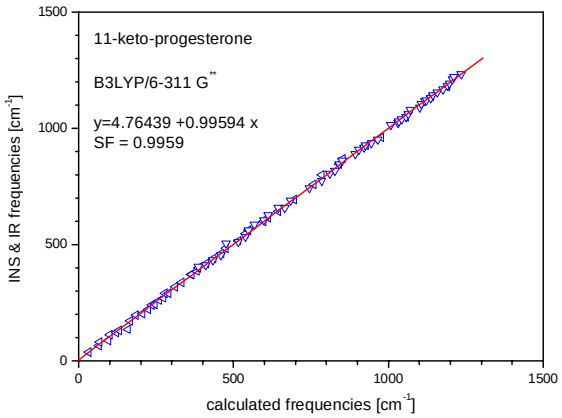

Fig. 3. Comparison of the experimental values of normal modes from IINS and IR spectra of 11 keto - progesterone with calculated ones by DFT method.

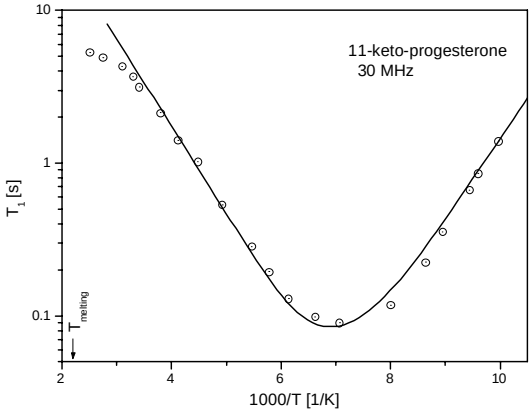

Fig.4. Temperature dependence of ^{1}H spin-lattice relaxation time of 11 –keto progesterone at 30 MHz.

Table 1. The calculated heights of barriers for reorientations of the methyl group about the C-C axis in 11-keto-progesterone compared with the experimental NMR data and IINS assignment.

Assignment of normal modes	IINS and IR frequencies of 11-keto-progesterone	Activation energy	Calculated activation energy [kJ/mol]		IINS and IR frequencies of progesterone	Activation energy [1]	Calculated activation energy [kJ/mol]
$\chi[CC(18)H_3]$	(203) (239)	12.5 ± 0.9	10.2		(141) *168* (170.3) (190) *224* (219.9) (220)	10.9±0.8	8.2
$\chi[CC(19)H_3]$	(203) (221) (239)	9.6 ± 0.9	6.0		*224* (220) *263* (252)	10.9±0.8	9.2
$\chi[CC(21)H_3]$	(111) (136) (141) (150)		1.4		(90) *102* (97) (110)	3.4	3.8

IINS frequency are printed in normal fonds, IR in italic

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Microscopic Structure of Liquid Na-Pb Alloys Studied by Neutron Diffraction

N.M. Blagoveshchenskii[1], V.A. Morozov[1], A.G. Novikov[1], D.V. Savostin[1], V.V. Savostin[1], A.L. Shimkevich[2]

[1]*State Scientific Center, Institute for Physics and Power Engineering, 249033 Obninsk, Russia*
[2]*Institute of Nuclear Reactors, Russian Research Center «Kurchatov Institute», 123182 Moscow, Russia*

Introduction

Liquid alloys of sodium and IVb elements (Sn, Pb) represent the subject of numerous macroscopic and microscopic investigations by different methods [1] including neutron diffraction [2, 3], reverse Monte-Carlo method [4], and molecular-dynamics (MD) simulation [5]. The interest in these systems arises from their structural micro-non-homogeneity concerned with possible cluster formation as a quasi-molecular group, Na_mMe_n (Me = Sn, Pb), with the tetrahedral atomic packing. The mentioned investigations have dealt with Na–Pb alloys containing lead of 20 at.% and more. So, it is of interest to understand the situation for alloys of lead concentration less than 20 at.%. There is also the practical interest to the binary Na–Pb system. 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.

Experiment

The neutron diffraction experiment was performed with DIN-2PI time-of-flight spectrometer [6] 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 1.5 at.%, and pure sodium as reference system at 700 K.

Results

The measurement procedure and primary data processing were standard for such a kind of experiments [7]. 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.

The angular differential scattering cross-sections were calculated as

$$d\sigma/d\Omega = (J_S/J_V)\left(d\sigma/d\Omega\right)_V N_V/N_S \qquad (1)$$

where J_S and J_V are the count intensities of the sample and standard vanadium sample, $(d\sigma/d\Omega)_V$ is the differential cross-section for vanadium, N_S and N_V are the numbers of sample and vanadium nuclei in neutron beam respectively. The static structure factor, $S(Q)$, related to differential cross-section as

$$S(Q) = (d\sigma/d\Omega)\, 4\pi/\sigma_{\text{coh}} \qquad (2)$$

where σ_{coh} is the coherent scattering cross section. The $S(Q)$ and radial distribution functions, $g(r)$, obtained for liquid Na–Pb alloys are shown in Fig. 1.

The experimental data on microstructure of the Na–Pb alloys we can compare with the results of MD simulation for the $Na_{0.98}Pb_{0.02}$ and $Na_{0.91}Pb_{0.09}$ alloys at 698 K [8].

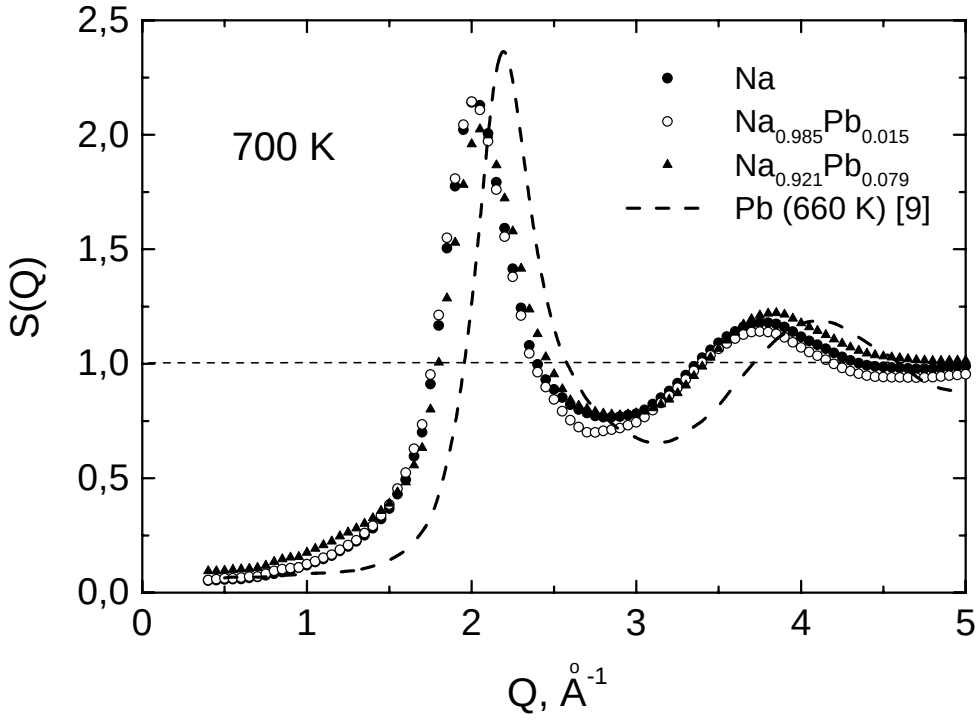

Fig. 1. The structure factors of liquid sodium and Na–Pb alloys.

Conclusions

1. The neutron diffraction experiment on pure sodium and liquid Na–Pb alloys with lead concentration of 1.5 and 7.9 at.% was performed. The static structure factors, $S(Q)$, and radial distribution functions, $g(r)$, are obtained.

2. Unlike the Na–Pb alloys with Pb concentration of 20 at.% and more [3], the prepeak in the small-Q region, which is usually connected to cluster forming, is not observed. But for the $Na_{0.985}Pb_{0.015}$ and $Na_{0.921}Pb_{0.079}$ some excessive intensity as to pure sodium is visible in this Q-region where some clusters formation is possible too [9].

3. The overall agreement between the experimental data and MD-results takes place.

4. From the analysis of MD results performed by the statistical geometry methods [8] it was concluded that changes of the liquid sodium microstructure at the addition of 2 and 9 at.% of lead specify on the clusterisation of impurity atoms as a colloid particles $(Na_2Pb)_n$. However, they have wide variation in size not united together at average distance. This fact causes the absence of the prepeak in the experimental $S(Q)$.

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Influence of Fe intercalation on phonon density of states of $TiSe_2$

A.N. Titov[1], S.G. Titova[2], A.N. Skomorokhov[3], V.A. Semenov[3]

[1]*Institute of Metal Physics UrD RAS, Ekaterinburg*
[2]*Institute of Metallurgy UrD RAS, Ekaterinburg*
[3]*Institute for Physics and Power Engineering, Obninsk, Russia*

Titanium diselenide $TiSe_2$ is a layered compound with the structural type of CdI_2, space group $P\bar{3}m1$, formed by a sequence of Se-Ti-Se sandwiches with octahedral coordination of Ti atoms by selenium. The gap between the sandwiches is available for occupation by intercalated atoms. In case of intercalation by transition and noble metals M the formation of covalent centres Ti-M-Ti has been observed, which may be considered as centres of lattice deformation (compression in perpendicular to layers ***c***-direction) and, at the same time, as the traps for free electrons [1]. It was shown that heating of the Fe_xTiSe_2 system above 550 °C leads to charge carrier delocalization [2]. The compounds of Fe_xTiSe_2, quenched from temperature higher than 550 °C remains metallic at room temperature [3]. Localization of charge carriers in Fe_xTiSe_2 at small concentration of iron $0<x<0.25$, and so, of impurity polarons, is the first order phase transition.

To study the charge carriers localization in Fe_xTiSe_2 inelastic neutron scattering experiment with DIN-2PI spectrometer [4] have been performed on $TiSe_2$, slowly and fast cooled samples of $Fe_{0.25}TiSe$. The powder samples were placed in thin aluminum foil container. Spectra have been measured at 15 detector groups between 28° and 134° at the initial neutron energy E_0 = 10.5 meV. The energy resolution, $\Delta E/E$, was ~6%. Calibration of the He^3 detectors was performed using the scattering from a standard vanadium sample. As a result the differential cross-section $\frac{d^2\sigma}{d\Omega dt}$ with respect to interval of time *dt* and solid angle $d\Omega$ was obtained. The standard treatment procedure, including corrections for background of empty container, efficiency of each detector has been applied for measured $\frac{d^2\sigma}{d\Omega dt}$ spectra, taking into account Jacobian for transformation from time to energy scale, $\frac{d^2\sigma}{d\Omega dE}$. Than the spectra of dynamic structure factor $S(Q,\varepsilon)$ have been obtained according to the following expression:

$$S(Q,\varepsilon) = \frac{4\pi}{\sigma_b}\frac{|\mathbf{k}_0|}{|\mathbf{k}|}\frac{d^2\sigma}{d\Omega dE}, \qquad (1)$$

where σ_b is the total bound atoms scattering cross sections per scattering unit, $\mathbf{k}_0$ and $\mathbf{k}$ are initial and final neutron wave-vectors, respectively Q is the modulus of the neutron momentum transfer $Q = |\hbar\mathbf{k}_0 - \hbar\mathbf{k}|$ and ε is energy transfer $\varepsilon = E_0 - E$. The generalized phonon density of states $G(Q,\varepsilon)$ have been derived according to:

$$G(Q,\varepsilon) = \frac{\varepsilon}{[n(\varepsilon)+1]}\frac{2m}{(\hbar Q)^2}e^{2W}S(Q,\varepsilon), \qquad (2)$$

were, m is mass of the scattering unit, $n(\varepsilon)+1$ is the Bose population factor, and W is an average Debye-Waller factor taken to be independent of Q. As a preliminary result, the neutron-weighted phonon density of states $G(\varepsilon)$ was obtained by averaging $G(Q,\varepsilon)$ over a number of Brillouin zones at the momentum transfer range of 1.1 $Å^{-1}$ <Q < 8 $Å^{-1}$ [5] without correction for multiple scattering and multiphonon contributions.

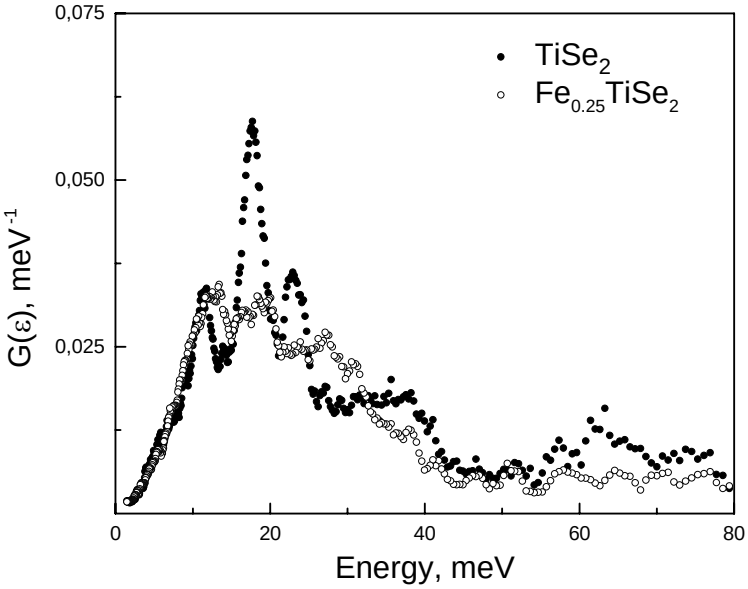

Fig. 1. The generalized phonon density of states in $TiSe_2$ and slowly cooled $Fe_{0.25}TiSe_2$

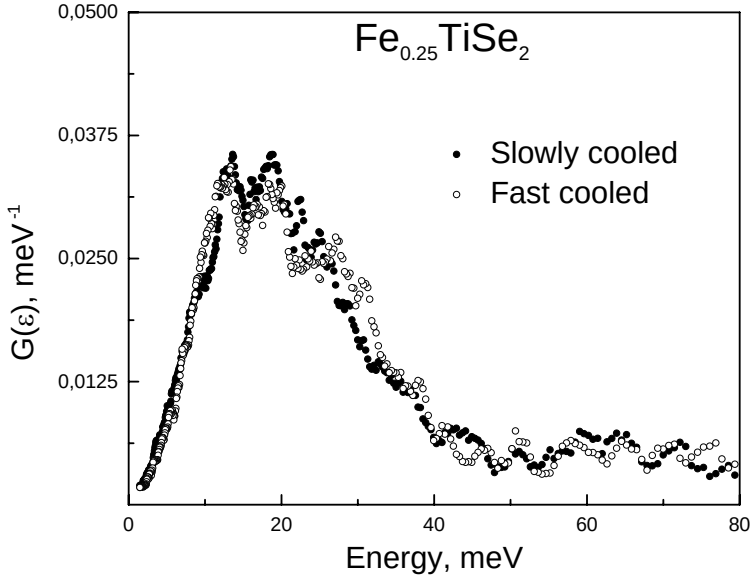

Fig. 2. The generalized phonon density of states in slowly cooled and quenched $Fe_{0.25}TiSe_2$

The generalized phonon density of states in $TiSe_2$ and slowly cooled $Fe_{0.25}TiSe_2$ are shown in Fig. 1. For $TiSe_2$ three well defined peaks at E=11.5, 17.7 and 23 meV and three more weak and broad maxima at ~6.3, 37 and 63 meV are visible. As a result of iron intercalation the broadening of the peaks at 11.5, 17.7 and 23 meV has been observed;

intensity in the low-energy part of the spectra (ε < 30 meV) increases, while at high-energy part (ε > 30 meV) decreases, the maximum at 63 meV vanishes in $Fe_{0.25}TiSe_2$.

The difference in $G(\varepsilon)$ of slowly and fast cooled samples of $Fe_{0.25}TiSe_2$ is clearly observed (Fig.2). At ε < 6 meV $G(\varepsilon)$ in slowly cooled sample is higher in comparison with quenched one, while at ε = 10–12 meV is much less. The peaks at $\varepsilon \sim$ 28 and 32 meV shift to the low-energy edge for slowly cooled sample. As we attribute slow cooling with a presence of polaron charge carrier, we can conclude that formation of polarons leads to a softening of phonon modes with $\varepsilon \sim$ 28 and 32 meV. These modes correspond to inter-layer phonons, so we come to the conclusion that formation of polaron state of charge carrier leads to a softening of just inter-layer phonon modes.

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EFFECT OF CnNO SURFACTANTS ON THE DOPC BILAYER THICKNESS IN UNILAMELLAR LIPOSOMES: SANS STUDY

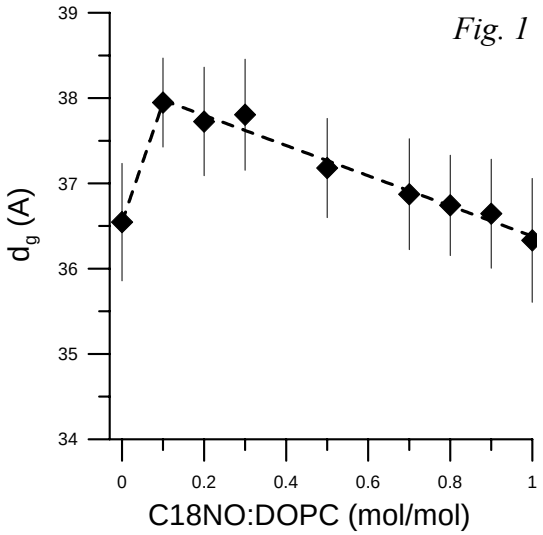
D. Uhríková[1], A. Islamov[2], A. Kuklin[2], F. Devínsky[1], I. Lacko[1], P. Balgavý[1]

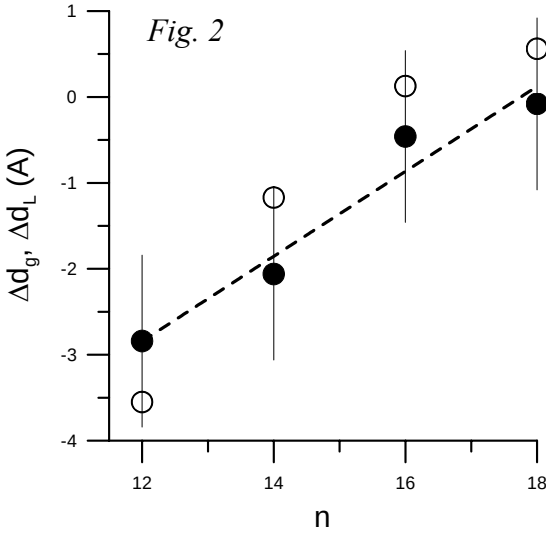
[1]*Faculty of Pharmacy, J. A. Comenius University, Bratislava, Slovakia*
[2]*Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia*

N-Alkyl-*N*,*N*-dimethylamine *N*-oxides (CnNO, *n* is the number of carbons in the alkyl substituent) are non-ionic surfactants at physiological values of pH [1]. C12NO is widely used for the solubilization of biological membranes, and for the isolation, purification and crystallization of membrane proteins [2,3]. CnNOs are also very potent bactericidal [4] and algicidal [5] agents. In the biological action and in various biochemical and biophysical applications of surfactants, their interaction with the phospholipid bilayer, the structural matrix of biological membranes, is of primary importance. In our previous SANS experiments, we have studied the C12NO effects on the bilayer thickness in unilamellar dioleoylphosphatidylcholine (DOPC) liposomes [6]. Here we extend this study to C12NO-C18NO homologs.

CnNO surfactants were prepared from corresponding *N,N*-dimethylakylamines by oxidation with hydrogen peroxide and purified as described in [7]. The methanol DOPC (Avanti Polar Lipids) and CnNO solutions were mixed to obtain the needed CnNO:DOPC molar ratio. The solvent was evaporated under a gentle stream of N_2 gas and its traces removed by a prolonged evacuation. D_2O was added and the mixture thoroughly homogenized. This dispersion was extruded 51 times through the Nucleopore polycarbonate filter with 50 nm pores using the LiposoFast Basic extruder (Avestin). In the dispersion of unilamellar liposomes thus prepared, the final DOPC concentration was 1 wt %, the pH value varied between 7 and 8. The dispersions were filled in the Hellma 2 mm quartz cells and the SANS curves were measured on the YuMO spectrometer at 25°C.

From the Kratky-Porod plot $\ln[I(Q)Q^2]$ vs. Q^2 of SANS intensity $I(Q)$ in the range of scattering vector Q values corresponding to $0.001\ Å^{-2} \le Q^2 \le 0.006\ Å^{-2}$, the bilayer radius of gyration R_g and the bilayer thickness parameter $d_g = 12^{0.5} R_g$ were obtained. A typical d_g dependence on the C18NO:DOPC molar ratio is shown in Fig. 1. It is seen, that after an increase of d_g at C18NO:DOPC~0.1 mol/mol, the value of d_g decreases with the increased C18NO concentration in the bilayer. Similar dependence was observed for the C12NO [6] and the other CnNO (n=14, 16) homologs (present work, not shown). This biphasic effect of CnNO could be caused by different locations of CnNO in the bilayer at low and high concentrations. Our previous spin label ESR studies [8] indicated that N-(1-methyldodecyl)-N,N-dimethylamine N-oxide (1MeC12NO) decreases the amount of *gauche* conformations in the hydrocarbon chains in the hydrophobic core of the bilayer bilayer at low concentrations; at increased concentrations, the amount of *gauche* conformations in the hydrocarbon chains gradually increased. This is consistent with the CnNO effects on the bilayer thickness. We have suggested [8] that the surfactant molecules are located predominantly in structural defects between phospholipid clusters at low concentrations and, after filling up these defects, the surfactant molecules penetrate into the clusters between lipid molecules, expand the bilayer laterally and decrease the bilayer thickness due to the mismatch between the surfactant and phospholipid hydrocarbon chain lengths. The present SANS results support this hypothesis. We have fitted the decreasing part of d_g vs. CnNO:DOPC molar ratio data by the linear function and calculated from the fitted function the change of bilayer thickness





parameter d_g as $\Delta d_g = d_{g0} - d_{g1}$, where d_{g0} and d_{g1} is the value of d_g at CnNO:DOPC=0 and 1 molar ratio, respectively. It is seen in Fig. 2 (full circles) that the most pronounced effect on the bilayer thickness exerts the CnNO homolog with the shortest alkyl chain length n=12. With the increasing alkyl chain length n the CnNO effect on the bilayer thickness diminishes. The SANS results in Fig. 2 (full circles) coincide within experimental errors with the bilayer thickness data recently obtained (Fig. 2, open circles, Δd_L) with the CnNO+EYPC lamellar phase at low hydration (H_2O:EYPC=12 mol/mol) by using the X-ray diffraction and the gravimetric method of data evaluation [9]. The dependence of the bilayer thickness change on the length of alkyl substituent seen in Fig. 2 is the experimental proof of the free volume model of surfactant – lipid bilayer interaction developed by our group [10,11].

Acknowledgements

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SMALL-ANGLE NEUTRON SCATTERING FROM HIGHLY STABLE WATER-BASED FERROFLUIDS

M.Balasoiu[1,2], M.V.Avdeev[1], V.L.Aksenov[1], D.Bica[3], L.Vékás[3]

[1]*Frank Laboratory of Neutron Physics,*
Joint Institute for Nuclear Research, Dubna, Moscow Reg., Russia.
[2]*Institute of Space Sciences, Bucharest, Romania*
[3]*Laboaratory of Magnetic Fluids,*
Center for Fundamental and Advanced Technical Research, Timisoara, Romania.

Ferrofluids (magnetic fluids) are stable dispersions of magnetic materials in liquids, which have been actively employed in different industrial and technical fields in the last thirty years [1]. An increase in the classes of carriers for producing ferrofluids widens the range of possible applications of these systems. The most stable ferrofluids are known among those based on organic non-polar solvents. In these systems the presence of a single layer of surfactants on the surface of magnetic particles is enough to avoid the particle aggregation in various external conditions including magnetic fields and temperature effects. Highest volume fractions of magnetic material, φ_m, for this type of ferrofluids achieve more than 20 % [2]. Stabilization of ferrofluids based on polar carriers is a more complicated problem, since the stabilizing surfactants should satisfy stricter requirements than in the previous case. On the one hand, they should possess sufficient chemical adsorption on the magnetic material, and on the other hand, they should be soluble in the polar carrier. The problem can be solved through the double stabilization method, when, after the surfactant of one type is adsorbed on the particle surface through the chemical adsorption, the surfactant of the same or another type (depending on adsorption properties) is adsorbed on the previous layer through the physical adsorption. This results in the so-called steric stabilization of colloidal particles. In recent years, a certain progress in the synthesis of stable polar ferrofluids with large volume fractions of magnetic materials using the double stabilization method (e.g. pentanol-based ferrofluid, $\varphi_m \sim 20$ %) has been achieved [3, 4]. In this connection, the structure of this type of ferrofluids and its comparison with that of non-polar ferrofluids is of current interest. It should be also pointed out that the development of biomedical applications of ferrofluids (e.g. cancer treatment with magnetic fluid hyperthermia [5]) requires stable biocompatible polar ferrofluids, first of all based on water, and the knowledge of mechanisms of stabilization in such fluids plays a crucial role in this field.

Here, we report about experiments on the small-angle neutron scattering (SANS) from new class of highly stable water-based ferrofluids. This class of ferrofluids was synthesized recently [4] in the Laboaratory of Magnetic Fluids, Center for Fundamental and Advanced Technical Research, (Timisoara, Romania). The stabilization of magnetite in deuterated water was achieved through the double layer of dodecylbenzenesulphonic acid (DBS). Our previous data for doubly stabilized water-based ferrofluids showed [6-8] that from the structural viewpoint a low stability of these fluids both in the absence and presence of external magnetic field is reflected in the formation of specific aggregation developing in time. The given kind of ferrofluids is distinguished by the high stability and comparatively large value of the maximal saturation magnetization, $M_\infty = 350$ Gs. The aim of the experiments was to reveal information about the structure of colloidal particles in this fluid in the absence of external magnetic field, as well as about the interparticle interaction at high values of volume fraction of magnetite. SANS measurements were made at the YuMO time-of-flight small-angle diffractometer of the IBR-2 pulsed reactor. The initial highly concentrated ferrofluid was

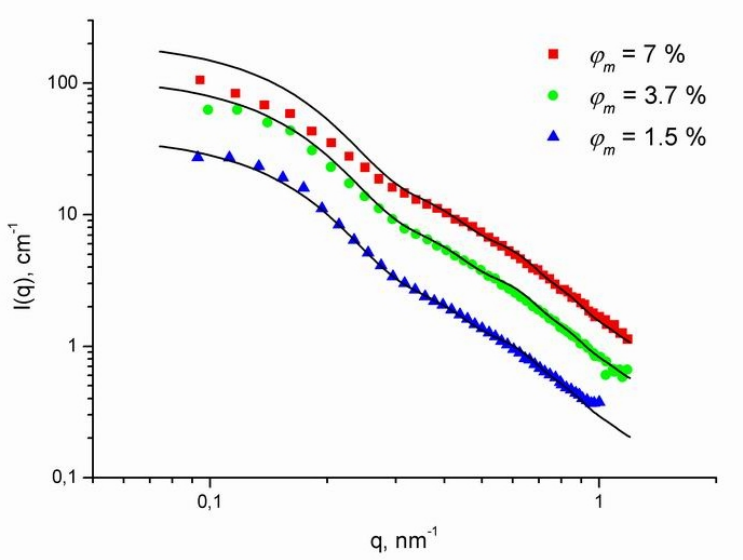

Fig.1. Experimental (points) SANS curves for ferrofluid Fe_3O_4/DBS+DBS/D_2O with different volume fraction of magnetite. Solid lines corresponds to the curves calculated according to the "core-shell" model.

dissolved down to several values of φ_m in the interval of 0.7 – 7 %. Several experimental SANS curves are presented in Fig.1. For the first time, the scattering from water-based ferrofluids of comparatively small magnetite content satisfies well the so-called core-shell model, when colloidal particles are considered as non-interacting homogeneous spheres (magnetite) covered with homogeneous shell (surfactant). The magnetite particles are assumed to be polydisperse with log-normal size distribution function, $D_N(R)$, with parameters R_0, S. The fits of this model to the experimental data are shown in Fig.1. The resulting parameters of the $D_N(R)$ function are R_0 = 4.8 nm, S = 0.45. The found value of the thickness of the surfactant shell is about 3.5 nm. It does not depend significantly on the particle concentration, and reflects a small interpenetration of the surfactant sublayers. It is interesting, that the model of non-interacting particles works well up to quite large values of the magnetite volume fraction, φ_m = 4 %, which corresponds to about 10 % of colloidal particle volume fraction. The analysis of the deviation of the model from the experimental data at high concentration (Fig.1) reveals a soft interaction between particles, which is explained by the extended surfactant shell.

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MOLECULAR DYNAMICS SIMULATIONS OF SOLUTION OF FULLERENE C60 IN CARBON DISULFIDE

A.Yu.Teterev[1,2], M.V.Avdeev[1], M.Kholmurodov[3], V.L.Aksenov[1,2]

[1]*Frank Laboratory of Neutron Physics,*
Joint Institute for Nuclear Research, Dubna, Moscow Reg., Russia
[2]*Physical Dpt., Moscow State University, Russia*
[3]*Laboaratory of Information Technology,*
Joint Institute for Nuclear Research, Dubna, Moscow Reg., Russia

In recent years fullerene solutions are actively studied. They exhibit some unusual properties such as non-monotonous behavior of temperature dependence of the solubility, solvatochromism and others [1,2]. The given work concerns the solution of fullerene C60 in carbon disulfide (CS_2), which possesses a comparatively high solubility, ~7.9 mg/ml. The system belongs [3] to a class of solutions where a peak in the temperature dependence of solubility is observed (T_{max} ~ 280 K). It has been studied [4 - 10] by different methods to reveal structural features of the fullerene in solution, as well as details of the fullerene-solvent interaction. The reported conclusions on some structural questions are contradictory. In particular, this concerns the size of C60 in CS_2. Thus, according to a number of experimental works on small-angle neutron scattering (SANS) the determined size is about 10 % more than that calculated from the known atomic coordinates of the fullerene molecule. Several assumptions to explain this difference can be made. The first one is the formation of the solvation shell around fullerenes due to their interaction with solvent molecules [7]. This assumption was checked carefully in [5] by measuring the concentration dependence of the scattering intensity and estimating the second virial coefficient of the solution. The conclusion was that this coefficient is close to zero, so there is no significant interaction between fullerenes and solvent molecules which would result in the solvation shell. Another reason is connected with the possible small aggregation, which is also suggested [11] for some fullerene solutions. If, in addition to monomers, there are dimers, trimers, e. c. in the solution and their fraction is not high, the character of the scattering curve is similar to that from the solution of monomers but with different parameters (in particular, the characteristic particle size) affected by the presence of aggregates. Finally, the discussed difference between the calculated and visible size of fullerenes in CS_2. can be caused by the so-called unacceptable volume effect. Usually, to calculate the volume of the dissolved molecule in a solvent the molecule of the latter is approximated by a sphere. From the covering of the dissolved molecules by these spheres the acceptable surface and volume unacceptable to solvent are estimated. It is clear that for the good precision the size of the solvent molecule should be significantly smaller in comparison with that of the dissolved molecule. This is not the case for fullerene solutions in CS_2, so that a specific organization of the CS_2 molecules close to fullerene surface would result in an effective increase of the unacceptable volume, and, hence, in visible size, of the fullerene. This assumption may be checked well by the molecular dynamics simulations.

Here, using molecular dynamics simulations (MDS) we consider the possibility of a specific arrangement of the solvent molecules at the interface with the fullerene. The pure CS_2 is well studied by means of MDS. The idea of the work is based on the fact that the characteristic size of the CS_2 molecule (~0.3 nm) is comparable with that of fullerene C60 (~1 nm), so that any interface organization of the CS_2 molecules different from that in bulk must

result in a significant difference between the interface and bulk molecular density of the solvent, and, hence, affects the visible size of the fullerene.

MDS calculations were performed with the program DL POLY [12]. First, they were made for the pure solvent basing on the work [13]. Then, after comparison of the results, they were repeated for the fullerene solution.

Initially, the basic cube in the calculations of 37.82 Å edge contained 512 molecules of CS_2. Toroidal boundary conditions were employed. The starting configuration was a simple cubic lattice of carbon atoms with randomized molecular orientations. Initial translations and rotational velocities were set equal to zero. Throughout the computation, CS_2 molecules were treated as rigid with bond length of 1.55 Å between carbon and sulfide atoms. Only the Lennard – Jones interaction were taken into account. The corresponding constants were taken from the previous work [13]. The forces and torques at a given molecule were summed in pairs up to cutoff radius R_c = 10 Å. The number density of liquid was taken to be ρ = 1.2 g/cm^3, which corresponds to the mean distance between carbons atoms of 4.73 Å. Time-step was set as $\Delta t = 10^{-4}$ ps. The whole computer run was taken 2870000 and 640000 turns for the first and second calculations, respectively. Temperature was stabilized with the Hoover thermostat at 293K.

For the fullerene solution the basic cube length were expanded up to 104 Å with the corresponding increase in a number of CS_2 molecules up to 10680. The central molecule was changed by the molecule of C60 fullerene, which corresponded to the fullerene concentration of about 1.2 mg/cm^3. The bonds in the fullerene molecule were considered as rigid. Other parameters of the calculations were the same like in the previous case [13].

The comparison of the resulting $g(r)$ functions for the pure CS_2 with those obtained previously [13] shows a good agreement between both calculations (Fig.1).

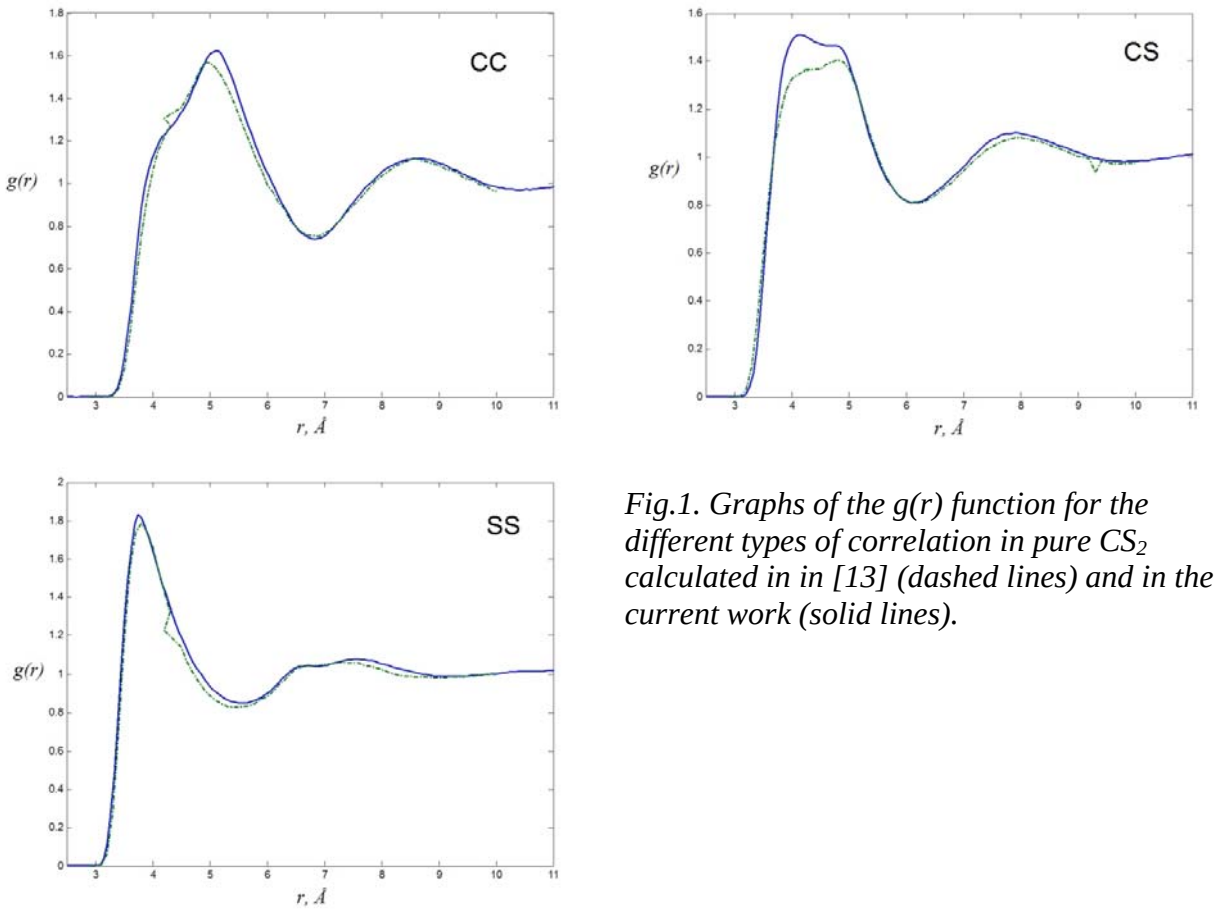

Fig.1. Graphs of the g(r) function for the different types of correlation in pure CS_2 calculated in in [13] (dashed lines) and in the current work (solid lines).

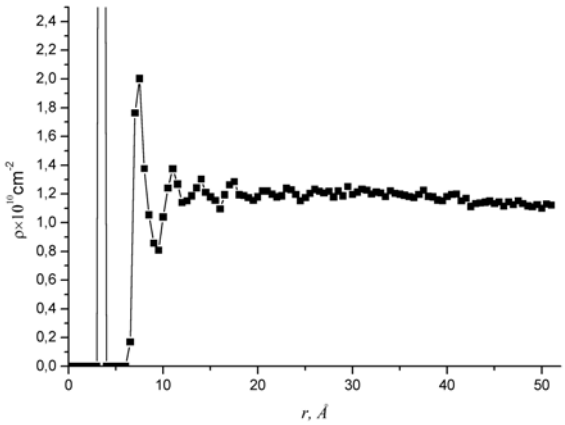

Fig.2. Profile of the scattering length density close to fullerene surface in solution of C60 in CS_2.

To analyze the organization of the solvent molecules at the interface with fullerene in C60/CS_2 the particle density functions were calculated with the origin in the center of mass of the fullerene molecule. A specific modulation of these functions close to the fullerene surface is detected. It is similar by nature to a short order seen in Fig.1 for the pure solvent. In experiments on the scattering from liquids the influence of such modulation takes place at large values of the momentum transfer (wide-angle diffraction) because of the small distances. But in the case of fullerene solution, the corresponding density fluctuations are connected with the size of fullerene molecule, and, hence, should contribute to the coherent scattering from fullerene in the SANS signal. The calculated scattering length density as a function of the distance from the center of fullerene molecules is plotted in Fig.2. According to calculations (Fig.2) the value of the bulk density at large *r*-values is about 1.20×10^{10} cm^{-2}, which is in good agreement with the value calculated from the physical solvent density, $\rho = 1.22\times10^{10}$ cm^{-2}.

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General trend in the changing of nuclear excited states structure

V.A.Khitrov, A.M.Sukhovoj

Laboratory of Neutron Physics, Dubna, Russia, 141980

The chief goal of experimental and theoretical investigations in low energy nuclear physics is the creation of a consistent model representation of the properties of nuclei in a specified interval of their excitation energy. In practice, it is necessary that the density ρ of the excited levels of nuclei in a specified interval of their quantum numbers together with the radiative strength functions k should be determined. Unfortunately, experimentalists have not been able to find a universal precise solution to the problem so far.

The new information about ρ and k appeared after the procedures for the determination of the intensities of two-step cascades as a function of the energy of their primary gamma-transition [1]:

$$I_{\gamma\gamma} = \sum_{\lambda,f} \sum_{i} \frac{\Gamma_{\lambda i}}{\Gamma_{\lambda}} \frac{\Gamma_{if}}{\Gamma_{i}} = \sum_{\lambda,f} \frac{\Gamma_{\lambda i}}{<\Gamma_{\lambda i}> m_{\lambda i}} n_{\lambda i} \frac{\Gamma_{if}}{<\Gamma_{if}> m_{if}}, \quad (1)$$

connecting the neutron resonance and specified low-lying levels of the studied nucleus and those for the extraction [2] from the data on the density of levels ρ and radiative strength functions

$$k = \Gamma_{\lambda i}/(E_{\gamma}^{3} \times A^{2/3} \times D_{\lambda}) \quad (2)$$

of cascade gamma-transitions, were developed.

A quite essential regularly observed difference between the observed and the calculated for 51 investigated up to now nuclei distributions of cascade intensity with the total energy $E_1 + E_2 = B_n - E_f$ (if the energies of their final level $E_f < 1$ MeV) shows that the existing representations and models of cascade gamma-decay need in serious correction.

From analysis of ρ and k yielded by studies of two-step cascades it follows that the structure of the wave functions of the excited levels is essentially different for their energy regions below and above $\sim 0.5B_n$. Consequently, the level density and the probability of their population (depopulation) differ significantly from those predicted on the basis of model representation of the nucleus as a purely fermion system (for example,[3,4]).

The specific character of the data obtained in [2] together with analysis of the conditions of the corresponding experiment calls for going over not only to more realistic models of level density ρ and radiative strength functions (2) (in a manner that would maximally reduce their dependence on the mass of the nucleus A) (of the type [5,6] and [3,7], respectively), but also to their more precise parameterization and further development.

Unfortunately, however, ρ and k obtained in accordance with [2] contain some unknown systematic error whose ordinary part is determined mainly by the inaccuracies of $I_{\gamma\gamma}$ determination. But in the present-day experiment it can be easily minimized to the small enough level not exceeding 5-20%.

In the present stage of technique development [2], the specific part of the systematic error is determined by possible existence of dependence of the strength function not only on the energy E_γ of a specified multipolarity quantum but also on the excitation energy E_{ex} of the decaying level , not accounted for in [2], i.e., by the existence of the function $k = F(E_\gamma, E_{ex})$ in place of the assumption that $\Gamma_{if}/\Gamma_i = F(E_\gamma)$ made when Eq. (1) was derived.

But we found the possibility to estimate the effect of the decaying level energy E_{ex} on the relative value of the radiative strength functions of gamma-transitions of equal multipolarity and energy. For all the investigated nuclei there is obtained a considerable volume of information about the intensities

$$i_{\gamma\gamma} = i_1 \times i_2 / \sum i_2, \tag{3}$$

that are energy-resolved in the spectra as pairs of peaks of individual cascades. Their parameters, including the most probable quanta ordering, are reliably extracted from the experiment up to the cascade intermediate level excitation energy 3-5 MeV with the help of an original technique of analysis created in Dubna that employs a numerical algorithm of resolution improvement providing for a maximum possible resolution of all the obtained spectra $E_1 + E_2 = const$ without loss of effectiveness [8].

From Eq.(3), taking advantage of the presently available data on $i_{\gamma\gamma}$, i_1 and i_2 the total population $P = \sum i_2$ of about 100 levels can be determined for the majority of the above enumerated nuclei to their excitation energy 3-4 MeV and higher. The difference between P and the intensity i_1 of primary transitions to each of the levels is equal to the sum of their population by 2-, 3-, etc.-quantum cascades.

Since at present, there is practically no possibility to determine experimentally the population of all, without exception, intermediate levels of two-step cascades even at their moderate excitation energies (due to the existing threshold of registration of the intensities $i_{\gamma\gamma}$, i_1 and i_2), it is reasonable to perform an experiment to calculation comparison for $P - i_1$ summed over a small interval of excitation energies. Such sums should be looked at as a lower estimate for each of the intervals.

The general regularities of changes in the level population with their changing excitation energy can be understood in three variant of calculations:

(a) the density of levels is predicted by the model [4], the strength function of E1-transitions is specified by known extrapolations of the giant electric dipole resonance in the region below B_n, and $k(M1) = const$ is specified by the normalization of $k(M1)/k(E1)$ to the experiment around B_n;

(b) ρ and k, that are obtained in accordance with [2] and reproduce exactly the intensity of two-step cascades as a function of energy of their primary transition, are used (at present, only for the final levels in the cascades with $E_f < 1$ MeV);

(c) a set of level density and strength function values is chosen to reproduce exactly ($\chi^2/f << 1$) the values of $I_{\gamma\gamma} = F(E_1)$, the total radiative width Γ_γ of the decaying compound state and the values of $P - i_1$ at the same time.

The realization of the variant (c) is possible in the iteration mode: for k obtained in

accordance with [2] there is selected some dependence function that would change the secondary gamma-transition strength function values with respect to that of the strength function obtained in accordance with [2] to enable the best reproduction of $P - i_1$. To this end, it suffices to multiply the strength functions of the secondary gamma-transitions to the levels below some boundary excitation energy U_2^{max} by the function h containing several narrow peaks. The dependence of their behavior on the excitation energy of the nucleus can be determined by analogy with the specific heat of ideal macrosystems in the second-order phase transition point as:

$$h = 1 + \alpha \times (ln(|U_c - U_1|) - ln(|U_c - U|)) \;\; if \;\; U < U_c, \tag{4}$$

$$h = 1 + \alpha \times (ln(|U_c - U_2|) - ln(|U_c - U|)) \;\; if \;\; U > U_c, \tag{5}$$

with some parameters $\alpha,\ U_1,\ U_2\ U_c$.

In the best variant tested by us, the amplitude α must grow from zero (linearly, for example) up to the maximally possible value shown in [9] as the excitation energy U decreases from $U = B_n$. The positions of the peaks, their amplitude and form are determined quite unambiguously by $P - i_1$. The population of any level whose number is l is determined by the equation:

$$P_l = \sum_m P_m \times \Gamma_{m,l}/\Gamma_m, \tag{6}$$

that depends on the population of all m higher-lying levels and on the branching coefficient of their decay. Although the data on the population depend on the two factors in the equation, the value of P for the different low-lying levels is mainly determined by the relationship between the partial widths of the secondary transitions populating them. Eq. (6) gives no other possibility to ensure an essential increase in the population of higher-lying levels.

The determined correcting functions are then included in the analysis [2] for the determination of ρ and k that exactly reproduce the cascade intensities taking into account an assumed difference between the energy dependence of the strength functions of the primary and secondary transitions in the cascade. If necessary, the cycle is repeated once at most if the hypothesis of linearly growing distortions in the value of $k(E1)$ and $k(M1)$ with increasing energy of the decaying levels is used and several times if the hypothesis of $\alpha = const$ is employed.

The effects of the different distorting factors for obtaines ρ and k for all set of investigated nuclei can be partially reduced by averaging them separately over even-even, even-odd and odd-odd compound nuclei. In the suggested variant, B_n equals unity for each of the nuclei and the level density is taken in the form of its relationship with the simplest interpolating function $const \times exp(\kappa E_{ex})$, whose parameters are fully determined by the densities of neutron resonances and levels in the excitation energy region around 1-2 MeV. Since k presented by (2) depends weakly on the mass of the nucleus, the sum of the strength functions of dipole transitions is directly averaged over nuclei with equal parity of nucleons. The averaging is performed for a set of a larger part of 40 nuclei for which ρ and k are determined by the method [4] as well as for the nuclei whose population

of individual levels is determined. As it is seen from Fig.1, in the first and the second variants the energy dependence $k(E1) + k(M1) \approx const$ for the primary transitions with $E_1 < 0.3B_n$ independently on the nucleus type. This confirms the principal validity of the basic representations of the model [3] for gamma-transitions from the compound states to the high-lying levels. Maximal possible values of $k(E1) + k(M1)$ are observed in the region $E_1 \approx (0.7 - 0.8)B_n$ and they decrease as the primary transition energy further increases.

As it is seen from Fig. 2, the function $R = const \times \rho \times exp(-\kappa E_{ex})$ has step-like structure with extremes in the region of $E_{ex} \sim 0.2$ and $\sim 0.8B_n$ and a minimum at about $0.5B_n$.

The attribute of the second-order phase transition is a sharp change in the internal properties of the investigated system as its energy changes. While quite a sharp change in the level density (i.e., in the specific heat of the nucleus, in fact) was earlier established experimentally in [2] with a sufficiently high reliability, the results of the performed analysis point to a sharp change in the reduced probability of gamma-transitions (primary, at least) in some, rather narrow, region of the levels of any nucleus excited by them.

The above reported results, that point to an essential increase in the radiative strength functions of secondary gamma-transitions for practically the same region of energies, can be considered as an additional independent proof of the existence of some region of excitation energies in the nucleus where a sharp change in the structure of the nucleus takes place. Presumably, it is a transition from domination of vibrational excitations to that of quasiparticle ones. Apparently, this can be interpreted as a phase transition from superfluid to ordinary state of such a specific system as nucleus. The effect is possibly associated with a breakup of the only pair of nucleons at excitation energies corresponding to a sharp decrease in the level density.

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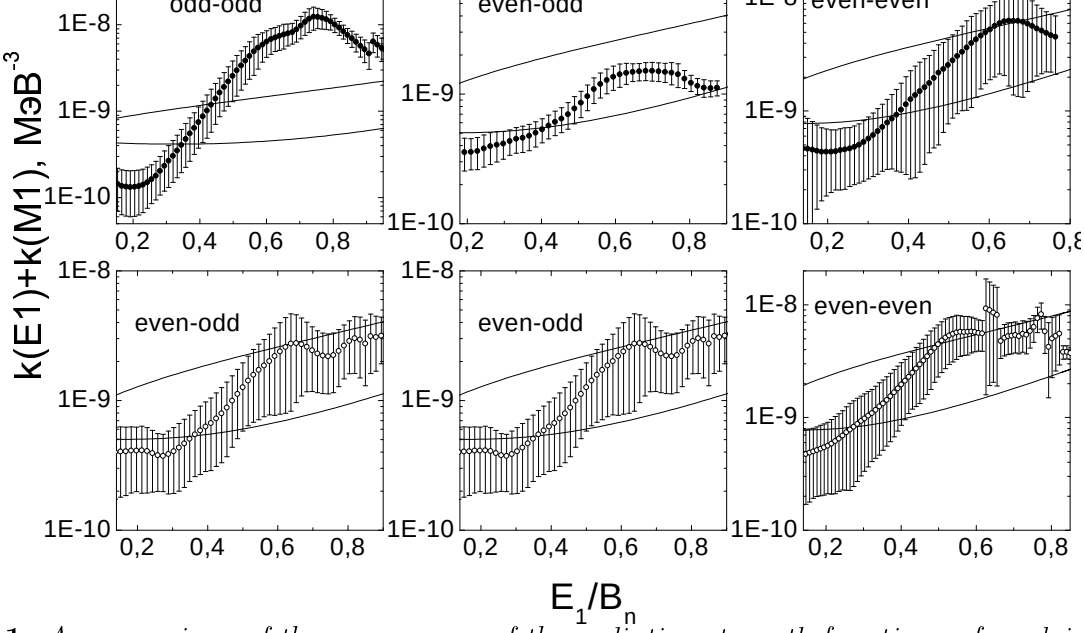

Fig. 1. *A comparison of the mean sums of the radiative strength functions of nuclei with the different parity of the number of neutrons and protons. Dark circles with errors - only nuclei for which the level population is determined. Open circles - all the nuclei for which the analysis [2] is performed without accounting for the difference between the energy dependence of the strength functions of the primary and secondary transitions. Upper curve - predicted by the model [10], lower curve –[3] under the assumption that* $k(M1) = const$

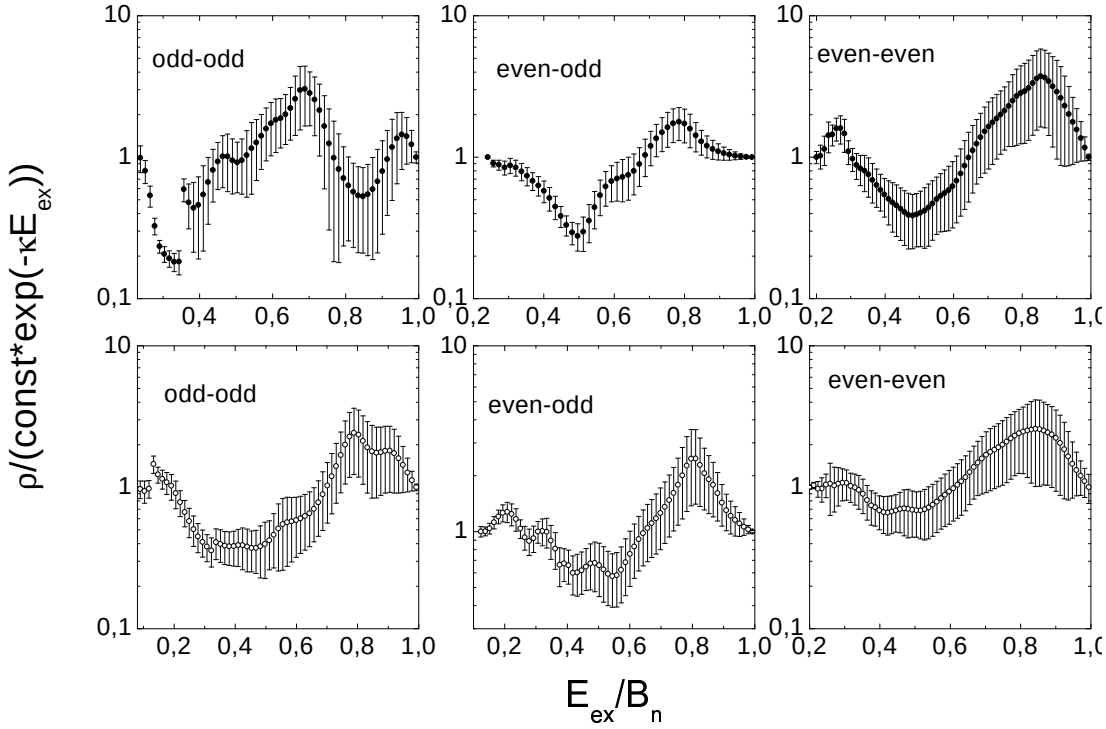

Fig. 2. Mean relative variations of the level density. The notation is similar to that for Fig. 1.

NEUTRONS FOR STYDING SYNTHESIS OF FINE CRYSTALLINE DIAMONDS

M.V. Frontasyeva, S.S. Pavlov, A.G. Dutov[1], V.A. Komar[1],
V.B. Shipilo[1], N.V. Shipilo[1], I.I. Azarko[2],

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

[1] *Institute of Solid State and Semiconductor Physics of NASB, Minsk, Belarus*

[2] *Belarusian State University, Minsk, Belarus*

The problem of finding optimal techniques to improve the structure of synthetic diamond crystals may be solved by way of comprehensive consideration of the processes of modifying the synthesis conditions and subsequent irradiation of fission spectrum by the neutrons [1]. Owing to the active influence of primary radiation defects on the microlevel, neutron irradiation can effectively form macroscopic properties of diamond crystals. Also, a supposition was put forward about the dependence of the change in a set of crystal properties on their containing of incidental admixtures, in particular, of aluminum. This investigation was continued at the synthesis of fine crystalline diamond powders in wider time intervals, and for high-energy processing the fission spectrum neutrons of pulsed reactor were used, which are more energy-hard in comparison with the neutrons of the steady state reactor.

Diamond crystals were obtained by the method of spontaneous synthesis at pressure P = 5.5 GPa and at temperature T = 1620 K in the Mn-Ni system with 0.15 % of copper added. The source of carbon was high purity graphite. The time of synthesis varied in the interval of 15–300 s with a pace Δt = 10 s, i.e., each experiment lasted for (15 + n Δt) s, where n =1, 2, …, 30. In the spontaneous process of synthesis during alternating periods of growth and dissolving of crystals, fine crystalline diamonds with sizes of granules from 315/250 to < 40 μm were forming. Extraction of diamonds and their sorting were performed in the way similar to the procedures described in the paper [2]. Irradiation of samples was conducted at the fast pulsed reactor IBR-2, FLNP JINR, Dubna, in the proportion of flux density of fast neutrons (≥ 1.0 MeV) to thermal neutrons equal to 3.34 [3]. Heating of the samples in the reactor channel did not exceed 30–40°C.The contents of paramagnetic centers and concentration of admixtures (Ni, Mn, Al) were determined in the same samples before and after irradiation by neutrons by the method of EPR-spectroscopy, by the roentgen fluorescent analysis, as well as by the epithermal neutron activation analysis at the IBR-2 reactor in Dubna [3,4].

With an increase of the time of synthesis and the crystal sizes in synthetic diamond samples a gradual decrease of paramagnetic centers of lattice point nickel is observed, which is accompanied by a decrease of width of the EPR line.

In Fig. 1 the dependence of lattice point nickel concentration on the crystal granule size before and after irradiation is presented for three times of synthesis. Basic features of the paramagnetic nickel behavior: a) decrease of the Ni^- concentration as a result of irradiation; b) presence of maximum; c) possible increase of the Ni^- concentration after irradiation (reverse distributions). During the alternating periods of growth of crystals and their dissolving in the process of long synthesis, concentrations of lattice point nickel and other admixtures decrease asymptotically but at certain moments, due to the intensification of crystal growth, after the stage of dissolving they may increase, simultaneously, maxima B and C are formed. Maximum A is probably connected with the loss of crystals of a very small size (R< 35 μm) during extraction and sorting.

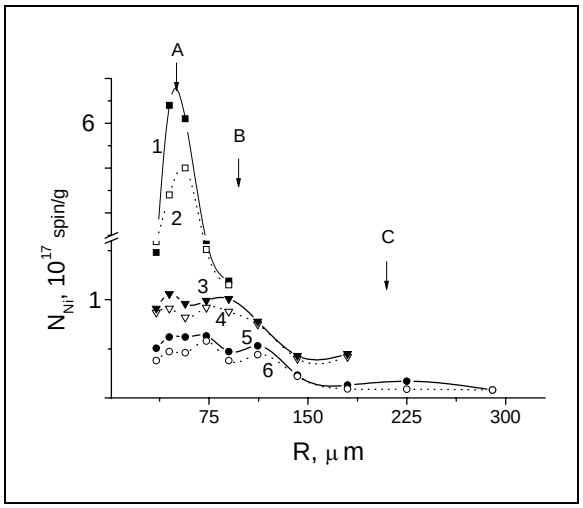

Fig. 1. Dependence of the Ni^- concentration on the size of crystals: *1, 2* – t_{syn} = 20 s; *3, 4* – t_{syn} = 90 s; *5, 6* – t_{syn} = 220 s before and after irradiation by neutrons, respectively

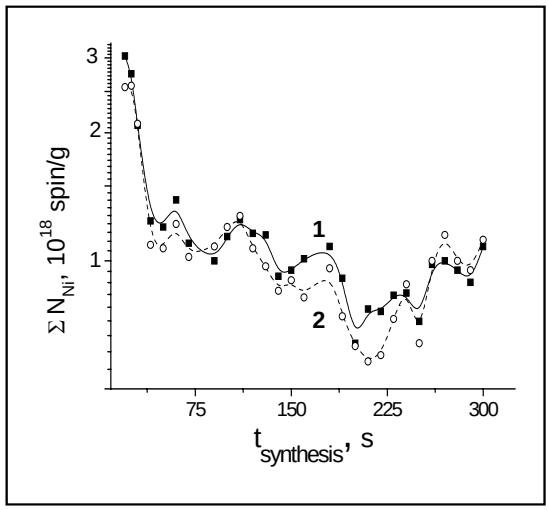

Fig. 2. Dependence of the integral Ni^- Concentration on the time of synthesis for diamond crystals with granularity from < 40 to 315 μm:
1, 2 – before and after irradiation by neutrons

As seen from Fig. 2, after the completion of initial phase of synthesis ($t_{syn} \geq$ 50 s), when the growth-dissolving stages occur, the concentration of paramagnetic nickel begins to vary near a decreasing mean value.

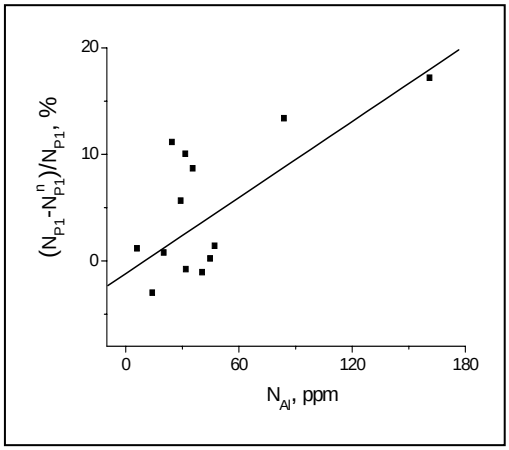

Fig. 3. Dependence of relative change in concentration of lattice point nitrogen (PC P1) after neutron irradiation on the contents of aluminum admixture in diamond crystals

Statistical processing of the obtained data concerning aluminum concentrations, paramagnetic centers (PC) P1 and PP-defects, as well as of concentration ratios $K = C_{Mn}/C_{Ni}$ for atoms of manganese and nickel, captured incoherently by joint borders of crystal and characterizing correlations between tangential and normal rates of crystal growth more distinctly than in the paper [1], showed the dependence of the Al N precipitate forming on the conditions of crystal growth. Figure 3 shows the dependence of the change of the PC P1 relative concentration, resulting from neutron irradiation, on the contents of aluminum admixtures in the crystals grown in the time interval 30-300 s. Stoichiometric correlation C_{Mn}/C_{Ni} = 1.50 prescribed initially by the composition of charge [5] is observed.

In Fig. 4 the relation between changes in concentration of PP and P1 defects for crystals with R < 40 μm is shown. As seen from the figure, the dependence is linear and is described by equation: $\Delta N_{PP} / N_{PP} = a + b(\Delta N_{P1} / N_{P1})$, (1) with α=0.895 (probability of the given accidental arrangement of points $p=3.7 \cdot 10^{-9}$). Here $\Delta N_{PP} = N_{PP} - N_{PP}^{(n)}$; $\Delta N_{P1} = N_{P1} - N_{P1}^{(n)}$ – change of concentrations of PP- and P1- centers resulting from irradiation, respectively.

For the crystals with R > 40 μm *b* coefficients in the equation (1), and also correlation coefficients decrease quadratically concurrently with the growth of crystal size.

Direct correlation with $\alpha = 0.61$ was discovered between the relative changes in concentration of PP-defects resulting from neutron irradiation and the contents of aluminum for the crystals with $K \leq 1.5$.

The results are also confirmed by the data obtained in the experiments with synthetic diamond crystals grown at various temperatures, at the same time $T_3 > T_2 > T_1$.

CONCLUSION

As the conducted investigations showed, the character of behavior of admixtures, such as nickel, aluminum, nitrogen and other elements, which are constantly present in crystals, their interaction with structural defects created, among other things, by neutron irradiation reflect accurately enough the processes occurring inside the reaction cell at spontaneous synthesis of diamond crystals and change of mechanism of crystal growth.

The influence of neutrons of fission spectrum on artificial diamonds is fairly strong and at defined doses is determined by the technology of crystal synthesis.

A similar nature of phenomena was detected taking place under the action of time and dimensional factors in the process of synthesis, as well as under the influence of neutron irradiation, in particular, a change of concentration of paramagnetic nickel in crystals. It was shown that the change in concentration of PP-defects is related to the change in concentration of lattice point nitrogen defects.

The obtained results make it possible not only to better understand the processes occurring in the course of spontaneous synthesis but also be used to obtain larger and more perfect crystals.

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NAA AND AAS FOR STUDYING ELEMENTAL CONTENT OF STAPLE FOODSTUFFS IN CENTRAL RUSSIA

M.V. Frontasyeva, S.F. Gundorina, A.V. Gorbunov[1], S.M. Lyapunov[1], O.I. Okina[1]

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

[1]Geological Institute of RAS, Moscow Russia

It is known, that out of 92 chemical elements, which are found in nature, 81 are found in human organism. 12 of them are the basic, or «structural», ones and constitute 99 % of all elements in the organism. These elements are H, O, N, P, S, Cl, Ca, K, *etc*. 1 % falls to the share of the rest elements, it is they that were named trace elements (TE). According to vital necessity for human organism, TE are subdivided [1–5] into the essential (Fe, I, Cu, Zn, Co, Cr, Mo, Se, Mn) ones; conditionally essential (Br, B, F, Li, Ni, V, Si) ones; toxic (Al, As, Cd, Pb, Sb, Hg, Be, Bi, Tl) ones and the rest, whose action on human organism is not clearly determined by now.

The aim of the present investigation is to assess the balance of TE intake by human organism. Central region of Russia was chosen as a standard, since up to 70 % of RF population has similar living conditions with a rather unified nutrition and purification system of drinking water.

To achieve this aim, the following tasks were solved in the course of the present study:

- quantitative and qualitative assessment of population food allowances;
- analysis of trace element composition in main foodstuffs consumed by the population of Central region of Russia;
- analysis of trace element composition in drinking water in waterwork;
- assessment of human organism's intake of TE.

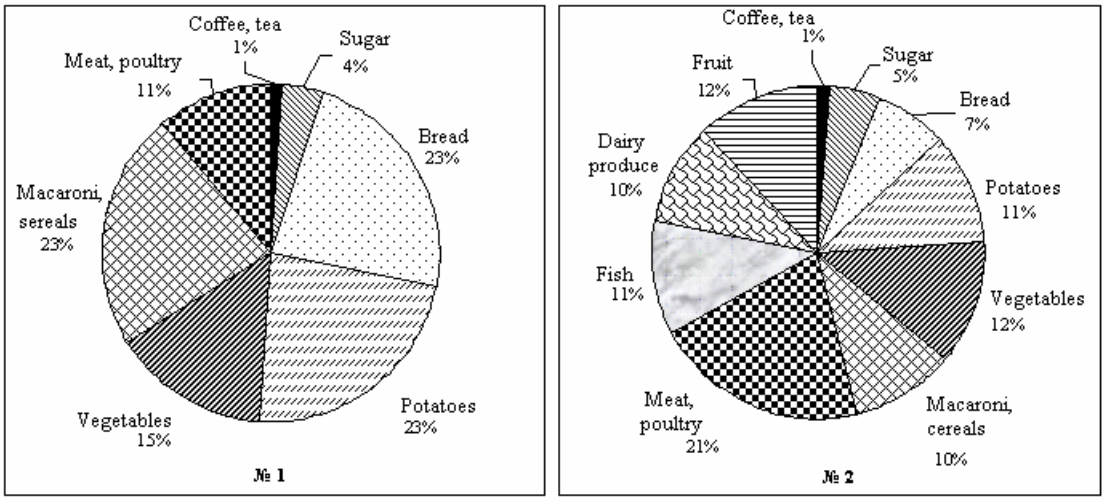
Sampling was carried out from retail trading network, farms and orchards located in the Central region of Russia. Sampling of vegetables and wild mushrooms was carried out directly in the areas where they grow in Moscow, Vladimir, Tver and Kaluga regions. River fish was fished up in rivers of Moscow, Tver and Astrakhan regions.

Epithermal neutron activation analysis using the REGATA analytical complex at the pulsed fast reactor IBR-2, FLNP JINR (Dubna), was applied to determine the content of 16 elements (Na, K, Ca, Cr, Mn, Fe, Co, Ni, Zn, As, Se, Br, Rb, Mo, Ag, Sb) in staple foodstuffs. Such elements as Cu, Cd, Hg, and Pb were determined by atomic adsorption spectrometry in the Geological Institute of RAS (Moscow) [6]

In the figure two different structures of food allowances are shown. Structure of the first food allowance, which we named the base one (food allowance № 1) constitutes a basis for the population, whose level of income corresponds to the living wage.

At present, in Russia such level of income has 23–27 % of population. Structure of the second food allowance was conditionally named the main one (food allowance № 2). Foodstuffs, which are included in it, are the main ones for the region population with an average level of income.

Multielement content of staple foodstuffs was studied in groups. On the basis of the obtained data the following features were revealed:



Structure of the base (№ 1) and the main (№ 2) food allowances

1. **Cereals, macaroni, bread:** The content of Cr, Ni in cereals and macaroni is high (close to or higher than the maximum allowable concentration (MAC)). The concentrations of Cu, Se, Sb are close enough to MAC. In bread an over MAC content of TE has not been observed. The content of Na, K, Ca, Cr, Br and Rb in white bread is 2-3 times higher, than in rye bread.
2. **Vegetables:** In leaf cultures, maize and legumes an over MAC contents of Cr and Ni were observed, also, the concentrations of Zn and Pb were close to them. The concentrations of Mg, Fe, Co, As, Br, Rb, La and Th were rather high. Also, enrichment with K and Ca was observed. It is important to note high Mo content in legumes.
3. **Fruit:** TE content does not exceed the RF norm.
4. **Mushrooms** (field mushrooms or *Agaricus campestris* and *Pleurotus ostreatus*): It was revealed that wild field mushrooms tend to accumulate heavy metals: Se content exceeds MAC 2 times, Cd – about 13 times, and Hg – 11 times. Concentrations of Ag, Au, Co, Cu, As and Pb are rather high. In wild Pleurotus ostreatus an excessive Cd concentration (10 times higher than MAC) was observed. Neither type of the mushrooms grown in artificial conditions demonstrates such tendencies.
5. **Seafood and fish:** For all these foodstuffs high contents of Na and Br are typical, freshwater fish is characterized by high Se content, and shrimp's meat – by As and Zn.
6. **Meat and dairy produce:** An over MAC content of TE was not detected, however, high Zn content was observed in all the subjects of inquiry, of Na and Ca – in meat, of Na, Fe, Br and Rb – in hen's eggs, and of Br – in dairy produce.
7. **Coffee, tea, sugar:** Tea is enriched with such elements as Ca, Cr, Mn, Fe, Co, Ni, Cu, Br, Rb, Cs, Pb, and coffee – K, Ca, Fe, Co, Ni, Cu, Zn, Br, Rb. Sugar is very poor in trace elements.
8. **Drinking water:** The results of study of TE content in drinking water in Moscow show that their concentrations are considerably lower than the world standards.

On the basis of the obtained experimental data, average rates of daily intake of the main TE have been calculated, also, a comparison with the existing literary data has been performed (Table).

Table. Human organism's intake of TE (mg/day)

El-t	Literary data		Experimental results	
	Need	Intake	Food allowance №1	Food allowance №2
Na	1400 - 1600	500 - 1500	800	1200 - 1600
K	2000 - 3000	2000 - 6000	8000	4000 - 5900
Ca	1000	1100	820	730 - 885
Cr	0.05 - 0.2	0.3	0.19	0.16
Mn	2 - 9	0.4 - 10	18	16 - 19
Fe	10 - 30	7 -8	33	16 - 18
Co	0.04 - 0.1	0.3	0.035	0.04 - 0.06
Ni	0.005 - 0.6	0.3 - 0.6	0.33	0.27 - 0.32
Cu	2 - 5	4 - 5	2.8	2.1 - 4.4
Zn	6 - 30	13	15	17 - 19
As	-	1 - 10	0.008	0.007 - 0.8
Se	0.1 - 0.15	0.06 - 0.33	0.13	0.15 - 0.24
Br	-	7.5	5.3	4.1 - 13
Rb	-	1.5 - 6	4.9	3.7
Mo	0.3	0.05 - 0.3	<0.05	0.24
Ag	-	0.07 - 0.1	<0.05	<0.05
Cd	-	0.01 - 0.2	0.007	0.005 - 0.11
Sb	-	0.002 - 0.1	0.06	0.02
Hg	-	0.001	<0.002	0.006 - 0.089
Pb	-	0.2 - 0.3	0.01	0.023 - 0.048

Note: (-) - stands for absence of data

CONCLUSIONS

As a result of the present study, trace element content of staple foodstuffs, which are typical for intake by the population of the Central part of Russia, has been determined. The data on TE content in Moscow drinking water are presented, their intake by human organism with the main food allowances has been assessed. Evaluating the results of the present study, we have come to the following conclusions.

1. An over MAC content of some TE, including the toxic ones, in various staple foodstuffs appears to be rather a widespread phenomenon. This may be due to several reasons: local or regional peculiarities of soil, on which agriproducts are grown, usage of fertilizers made from phosphorite (As, Cd, U), usage of leaded gasoline (Pb), ecological reasons. However, the main reason, in the authors' opinion, is the difficulties in development of effective systems of monitoring of TE content in staple foodstuffs.
2. The poorest TE content is in fruit and sugar, the richest TE content is in wild mushrooms, seafood, fish, vegetables (especially maize, legumes and leaf cultures).
3. On assessing the results of human organism's intake of TE with food allowances № 1 and 2, to our mind, we obtained rather paradoxical results. It proved to be that the most optimal is TE intake with food allowance № 1, which corresponds to the living wage and is poor concerning the diversity of foodstuffs. Intake of all the studied TE is within the need. At the intake of a more diverse food allowance № 2 a violation of balance of TE intake may occur (an increase in the intake of essential and toxic TE, while the intake of certain TE may be close to the toxicity edge).

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EPITHERMAL NEUTRON ACTIVATION ANALYSIS FOR FRESHWATER ECOSYSTEM MONITORING: THE RYBINSK RESERVOIR CASE STUDY

M.V. Frontasyeva, D.F. Pavlov[1] and S.S. Pavlov

Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia
[1] I.D. Papanin Institute for the Biology of Inland Waters of RAS, Russia

An increasing anthropogenic impact on the environment requires relevant monitoring systems to be developed to meet the challenges of sustainable environmental management [1].

The Rybinsk Reservoir served as a model of freshwater ecosystem. Some parts of this man-made lake are subjected to chemical emissions from numerous industrial enterprises. Most potent sources of environmental contamination to this man-made lake, fresh water supply of Moscow, are the cities of Rybinsk and Cherepovets, the latter known for its largest in Europe steel producing plant.

Multi-element epithermal neutron activation analysis (ENAA) was used to examine levels of chemical elements in the key components of a freshwater ecosystem – bottom sediments, bivalve mollusks and fish tissues – collected in the sampling sites shown in Fig. 1.

Fig. 1. Sampling sites

The reservoir's areas adjacent to the cities are characterized by high level of sediment and biota contamination with heavy metals [2, 3]. During the last years high concentrations of mercury were revealed both in bottom sediments and in fish species [4]. In contrast, other parts of the reservoir are comparatively clean (sampling site 10).

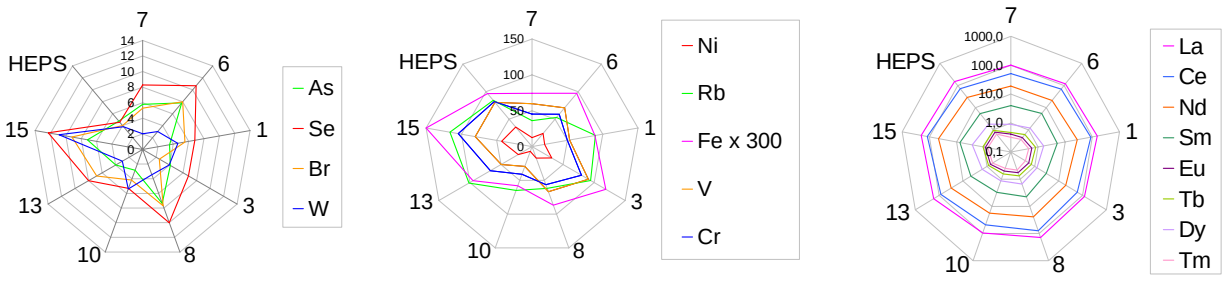
A total of 34 elements were determined: Na, Mg, Cl, K, Ca, Sc, V, Cr, Mn, Fe, Ni, Zn, As, Se, Br, Sr, Rb, Sb, I, Cs, Ba, La, Ce, Nd, Sm, Eu, Tb, Dy, Tm, Hf, Ta, W, Th, and U. As for lanthanides, until last decades a point of view prevailed about their biological inertness and low toxicity. As a result, no appropriate monitoring system for these elements is developed yet.

This means that the basic regularities of environmental behavior of these elements, key points of their cycles in aquatic ecosystems, as well as useful biondicator species, are unknown. Recent studies showed that at least some of REE are noticeably toxic for aquatic biota [5], thus necessitating developing of the monitoring system for these «new» potential pollutants and search for appropriate bioindicators. ENAA is particularly advantageous for determination of trace elements that have large activation cross-section (resonance integrals) at specific energies in the epithermal energy region [6]. NAA has the other advantage of not requiring the dissolution of samples, and thus has no difficulties associated with incomplete digestions or the possibility of introducing contamination by the chemicals applied.

Bottom sediments, bivalve mollusks (mixed samples of two hardly distinguishable species, *Dreissena polymorpha* and *D. bugensis*) and different types of fish (non-predatory bream, roach, and predatory zander, perch, *etc*.) were collected during summer expedition aboard of research vessel. The samples were stored in freezer at -18^{o} C before processing. After defrost in laboratory they were dried in thermostat at 90^{o} C to a constant weight and grinded with jasper mortar. Samples of about 200 mg (bottom sediments) and 500 mg (mollusks and fish) were packed in aluminum cups for long-term irradiation and heat-sealed in polyethylene foil bags for short-term irradiation. The description of irradiation channels and pneumatic system of the reactor IBR-2 FLNP JINR is given elsewhere [7]. To determine the short-lived isotopes, samples were irradiated for 5 min and measured twice after 3-5 and

20 min, respectively. Long lived isotopes were determined after irradiation for 4 days and then measure twice after 4-5 days of decay for 45 min and after 20 d of decay for 3 h, respectively. Data processing and element concentration determination was performed on the basis of certified reference materials and flux comparators, using software developed in FLNP, JINR.

As follows from the results obtained for bottom sediments, the concentration of most of elements varied insignificantly at different sampling sites. However the concentrations of such elements as As, Se, Br, W (Fig. 2, a) and Fe, Rb, Cr (Fig. 2, b) are the highest at the sampling site 15, i.e. moth of the Volga River. The concentrations of V and Ni are the highest at HEPS, the closest to the town of Rybinsk. The concentrations of lantanides (Fig.2, c) are practically the same at all sampling sites.



a) b) c)

Fig. 2. Distribution of some selected element concentrations in the bottom sediments (ppm) at the sampling sites 1, 3, 6, 8, 10, 13, 15 and HEPS

To make the results obtained visual, GIS technology was used for creating maps of distribution of elemental concentrations in bottom sediments. Examples for Mn, Fe, and Cr are shown in Fig. 3.

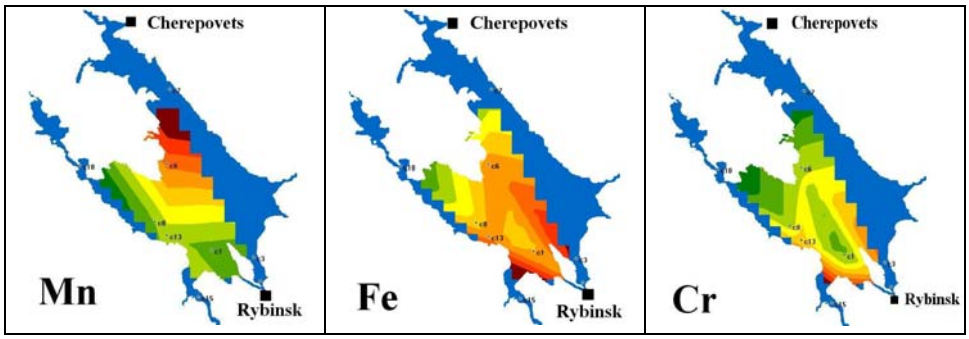


Fig. 3. Extrapolated distribution maps of Mn, Fe, and Cr concentrations in bottom sediments of the Rybinsk Reservoir. The green color corresponds to low concentrations, the red one to the highest

The analysis of chemical composition of mollusk and fish tissues revealed that in fact all elements found in the bottom sediments are observed also in biota although in varying concentrations. This evidences that elements analyzed, including lanthanides, are readily available for bivalve mollusks and fish. The concentration levels of lanthanides determined in the sediments and biota from the Rybinsk Reservoir are close to those from the Netherlands discussed in [6]. The mean concentrations of some selected elements in sediment samples, fish muscles and liver, bivalve mollusks shells and soft tissues (mantle) of mollusk and fish from the Rybinsk Reservoir are given in Fig. 4.

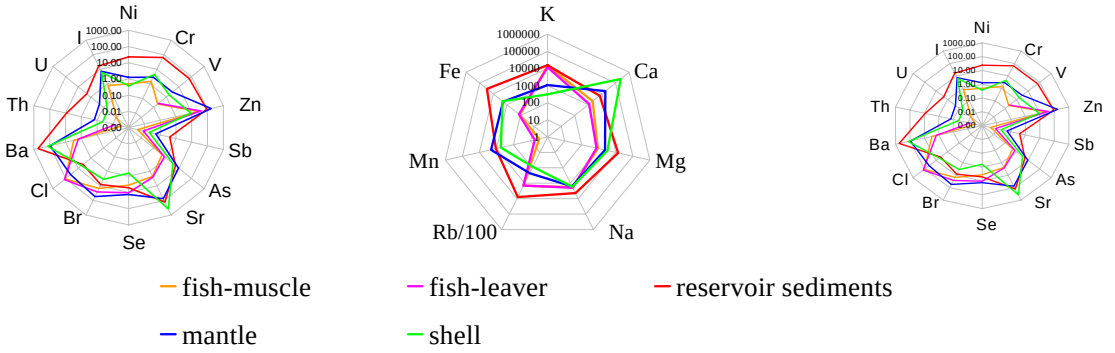


Fig. 4. Mean concentrations of some selected elements in samples of bottom sediment and different mollusks and fish tissues

The concentrations of Rb, Sm, Cs, Eu, Hf, Nd, Lu, Tb in sediment samples are higher than those in biota. Similar pattern is observed for most of elements besides Ca, Cl, Br, Se, Sr, Zn. This indicates that the first group of elements including some lanthanides is less bioavailable for the studied organisms. For these elements bottom sediments could serve as an effective environmental monitor. Among the organisms and organism tissues studied, bivalve mollusk soft tissues could best serve for the monitoring purposes since concentrations of majority elements analyzed (including lantanides) in these tissues were highest with only a few exceptions. This is quite understandable taking into the account bivalve filtration feeding and ability to accumulate many elements and substances.

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ENAA AND AAS FOR ANALYSIS OF SURFACE SOIL: EXAMPLE FROM THE THRACE REGION, TURKEY

S. V. Demkina, M. V. Frontasyeva, Mahmut Coşkun*, Münevver Coşkun*, E. Steinnes**

Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research
141980 Dubna, Moscow Region, Russia
**Çanakkale Onsekiz Mart Üniversitesi Sağlık Hizmetleri Meslek Yüksekokulu, 17100 Çanakkale, Turkey*
***Department of Chemistry, Norwegian University of Science and Technology, NO-7491, Trondheim, Norway*

The soil, a main part of the terrestrial ecosystem, is a habitat for a great number of organisms. At the same time it is, open to influence from a number of human activities. Among the most disturbing factors is the surface pollution with toxic metals from a variety of sources. In order to objectively assess the influence of this factor however the geochemical baseline concentrations of the metals concerned must be known.

In the Thrace region, the European part of Turkey, including the the highly populated city of Istanbul, this information is not available. The present study was therefore undertaken to fill this gap for this region, which is subject to rapid population growth and affected by intense agricultural and industrial activities.

An area of 24 000 sq. km was subdivided according to a 20×20 km grid and surface soil samples were collected in September 2001 within each of the resulting 73 squares. The samples were subjected to epithermal neutron activation analysis (ENAA) at the reactor IBR-2, Dubna, and to flame and graphite furnace atomic absorption spectrometry (AAS) in Trondheim.

Epithermal neutron activation analysis has shown to be a powerful technique for the multi-element determination of a great number of elements in soil samples over a large range of concentrations in soil samples with satisfactory sensitivity and accuracy [1]. By ENAA in combination with AAS a total of 35 elements were determined: 29 elements (As, Ba, Br, Ca, Cd, Ce, Cr, Cs, Eu, Fe, Hf, I, In, K, La, Mn, Mo, Na, Nd, Rb, Sb, Sc, Sm, Sr, Ta, Tb, Th, Ti, U, and V) by ENAA as described elsewhere [2], and 6 elements (Pb, As, Cd, Cu, Zn and Ni) by AAS.

Descriptive statistics for the determined elements is given in Table 1 along with the global mean values (3). For a majority of the elements the Thrace soil medians are in close agreement with the word medians. Multivariate statistics (VARIMAX rotated principal component analysis (PCA)) was applied to the data set to identify and characterize different sources of the elements. As shown in Table 2, five different factors were defined:

Factor 1 (Ce, Eu, La, Mn, Nd, Sm, Ta, Tb, Th, U) represents a lithogenic component. The distribution pattern of factor 1 shows no relation with settlement areas.

Factor 2 (Al, Co, Cr, Cs, Fe, Mg, Ni, Ti, Zn) may reflect a combination of industrial pollution and a lithogenic component.

The combination of elements associated with factor 3 (As, Ca, Cd, Cu, Pb, Sb, W) indicates pollution from industries and other anthropogenic activities.

Factor 4 (Br, I, K, Na) may indicate contribution to the soils from the atmospheric deposition of marine salts.

Factor 5 (Ba, Rb, Sr) is interpreted as an additional lithogenic component.

Contour maps for the elements of interest for the entire studied area were constructed using GIS (geographic information system) technology, as shown in Fig.1. SURFER 6.0 software with kriging algorithm was used to interpolate the data. Except for distinctly higher levels of Pb, Cu, Cd and Zn in areas near Istanbul the observed distributions seem to be mainly associated with lithogenic variations.

Table 1. Statistical analysis (mean, median, range) of the Thrace region soil data and world medians for the determined elements

	Mean	Median	Range	World median*
As	8	7	1.9-51	6
Ba	550	490	240-1160	500
Br	8	6	0.1-30	10
Ca	30700	16100	1750-164700	15000
Cd	0.2	0.1	0.03-1.7	0.35
Ce	69	64	30-150	50
Co	11	10	1.5-27	8
Cr	173	93	20-830	70
Cs	4.0	3.4	1.4-12.8	4
Cu	20	16	1.8-167	30
Eu	0.8	0.8	0.2-1.6	1
Fe	26900	27100	5800-55400	40000
Hf	5.4	5.0	2.2-10	6
I	8.5	8.0	2.2-22	5
In	0.4	0.4	0.09-0.7	1
K	20100	19100	8700-46700	14000
La	26	25	11.5-59.7	40
Mn	600	467	62-3760	1000
Mo	0.6	0.5	0.08-4.6	1.2
Na	7800	7700	1400-21700	5000
Nd	24	23	12-50	35
Ni	50	36	2.6-249	50
Pb	33	19	4.8-968	35 (12**)
Rb	93	89	35.5-186	150
Sb	0.9	0.6	0.2-6.7	1
Sc	10	10	3.5-20	7
Sm	5.6	5.4	2-13	4.5
Sr	178	149	44-543	250
Ta	1.2	1.0	0.4-2.2	2
Tb	0.8	0.7	0.3-1.4	0.7
Th	9	9	4-24	9
Ti	3700	3800	1500-6800	5000
U	2.6	2.3	1.3-5.5	2
V	78	80	18.6-170	90
Zn	45	45	6-165	90

*Values from Bowen (1979);**prior to global contamination

Table 2. Results of principal component analysis

Rotated Component Matrix Component					
	1	2	3	4	5
% of Variance	21.7 %	19.1 %	12.0 %	8.3 %	6.3 %
As	0.153	0.088	**0.861**	0.132	-0.103
Ba	0.141	-0.209	-0.249	-0.321	**0.767**
Br	0.448	0.173	0.198	**0.601**	-0.039
Ca	-0.144	0.293	**0.539**	0.248	0.182
Cd	0.497	-0.052	**0.499**	0.306	-0.072
Ce	**0.917**	0.163	0.091	0.118	0.100
Co	0.304	**0.759**	0.056	0.305	-0.090
Cr	-0.142	**0.576**	-0.261	0.317	0.015
Cs	0.469	**0.542**	0.215	0.113	0.158
Cu	-0.111	0.294	**0.846**	0.152	0.039
Eu	**0.687**	0.387	-0.063	0.142	0.173
Fe	0.321	**0.848**	0.156	0.188	0.034
Hf	0.364	-0.290	-0.353	-0.064	0.021
I	0.318	0.220	0.164	**0.670**	0.016
In	0.054	-0.112	0.279	-0.036	0.430
K	0.081	-0.158	-0.141	**-0.707**	0.504
La	**0.927**	0.141	0.092	-0.029	-0.027
Mn	**0.617**	0.217	0.145	0.026	-0.004
Mo	0.292	0.086	0.455	-0.159	-0.058
Na	-0.180	0.143	-0.349	**-0.665**	0.098
Nd	**0.791**	0.234	0.020	0.234	0.148
Ni	-0.133	**0.793**	-0.049	0.270	-0.083
Pb	-0.215	-0.039	**0.676**	0.127	0.161
Rb	0.422	-0.008	-0.103	-0.252	**0.755**
Sb	0.208	0.011	**0.863**	0.080	-0.104
Sc	0.338	**0.893**	0.110	0.013	0.036
Sm	**0.882**	0.245	0.052	-0.055	-0.038
Sr	-0.191	0.206	0.010	0.222	**0.561**
Ta	**0.747**	0.121	-0.030	-0.044	-0.089
Tb	**0.737**	0.460	-0.009	0.218	0.084
Th	**0.713**	0.221	0.013	0.144	0.392
Ti	0.382	**0.786**	0.102	-0.048	-0.223
U	**0.650**	0.092	0.184	-0.509	-0.011
V	0.291	**0.815**	0.239	0.015	-0.187
Zn	0.416	**0.568**	0.463	0.280	0.082

Extraction Method: Principal Component Analysis
Rotation Method: Varimax with Kaiser Normaliza tion. Rotation converged in 12 iterations.

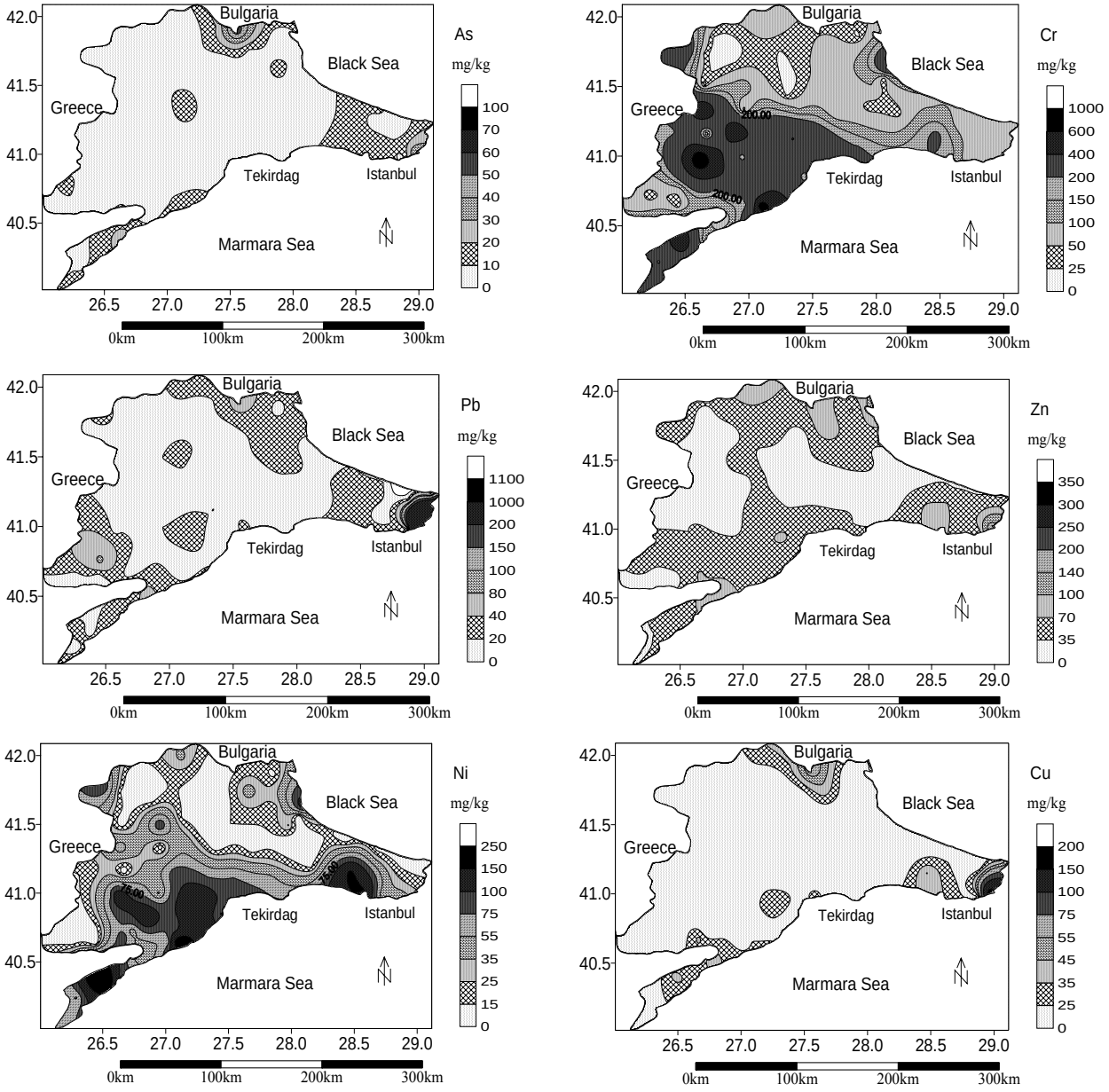

Fig. 1. Spatial distribution of As, Cr, Cu, Ni, Pb, and Zn in theThrace region, Turkey

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USE OF ENAA TO STUDY METAL POLLUTION IN THE VICINITY OF THERMAL POWER PLANTS IN CENTRAL RUSSIA

E. Ermakova, M.V. Frontasyeva and E. Steinnes[1]

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

[1]*Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway*

The combustion of fuel (coal, gas, crude oil) in thermal power plants (TPP) is a major source of atmospheric pollution with heavy metals [1, 2]. The moss biomonitoring technique is used here for the estimation of metal deposition in the vicinity of thermal power plants in Central Russia.

Moss samples (*Pleurozium schereberi*) were collected at 15 sites around the brown-coal fired Cherepetskaya TPP, Tula Region, and at 40 sites around the gas/crude oil fired Konakovo TPP, Tver Region. Samples in background territories of each region were obtained as well. The sampling procedure was similar to that used in the European project «Atmospheric heavy metal deposition in Europe» [3].

Epithermal neutron activation analysis was performed at the IBR-2 reactor as described elsewhere [4]. A total of 26 elements were determined (Na, Al, Cl, K, Ca, Sc, V, Cr, Mn, Fe, Co, Ni, Zn, As, Br, Rb, Sr, Sb, Cs, Ba, La, Ce, Sm, Tb, Th, U) using the reference materials IAEA-336 (lichen) and SRM 1575 (pine needles) for quantification.

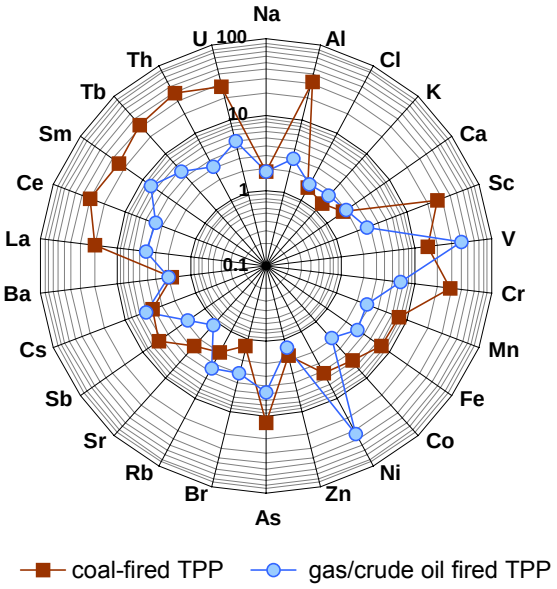

Fig.1. Ratios between element concentrations (mg/kg) in moss from the sampling site nearest to the TPP and the corresponding local background level

The concentration levels in moss at the most exposed sites are shown relative to the background levels in Fig. 1. As follows from the circular diagram, the concentrations of practically all elements exceed the local background levels for both TPP.

For some specific elements this excess is more significant than for others: the concentrations of V and Ni in moss collected in the nearest vicinity of the gas/crude oil-fired power plant (dots) are 30–40 times higher relative the corresponding background levels. Similarly the concentrations of As, Th, U and rare-earth elements in samples collected near the coal-fired power plant (squares) are more than 20 times higher than the background levels of these elements.

Concentration gradients of the above mentioned elements *versus* distance from the TPPs are shown in Figs. 2 and 3.

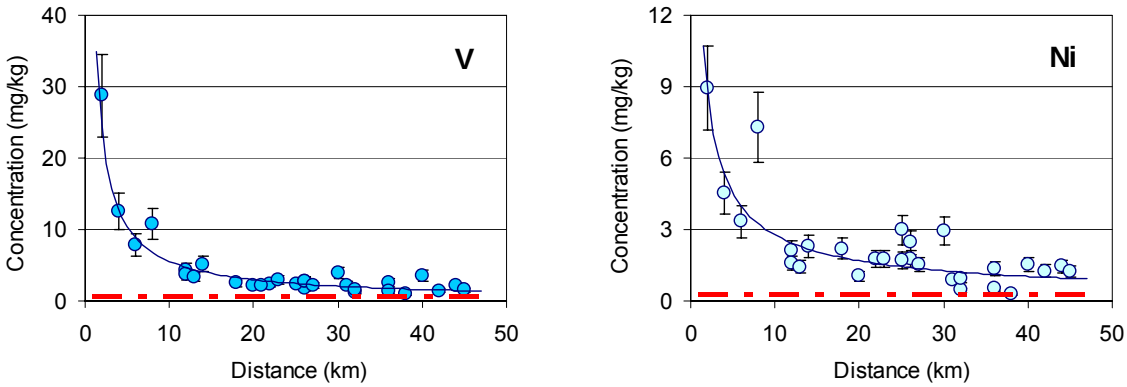

Fig. 2. Gradients of V and Ni concentrations in moss *versus* distance from the gas/crude oil-fired Konakovo TPP (dashed line is the background level)

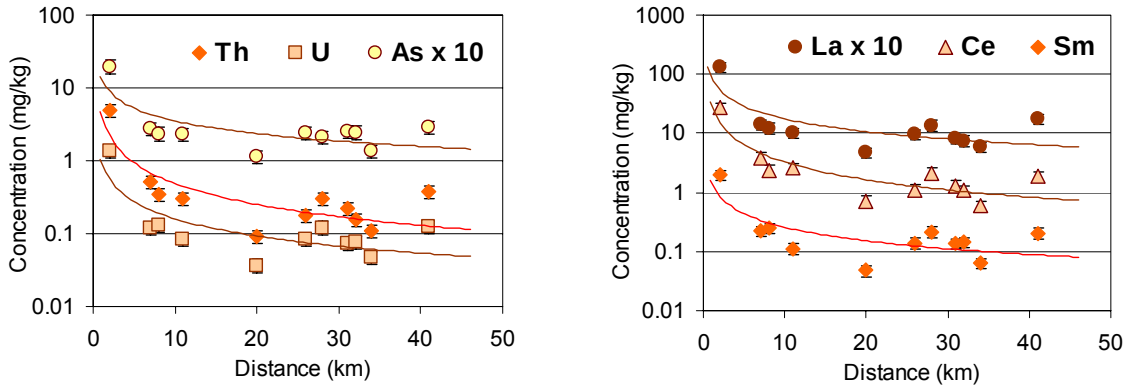

Fig. 3. Gradients of element concentrations in moss *versus* distance from the coal-fired Cherepetskaya TPP

The concentrations of these elements in moss decrease rapidly with distance from the source following a power trendline $y=ax^b$. Its parameters are shown in Table 1.

Table 1. Parameters of a power trendline and R^2* for some selected gradients of elemental concentrations in moss *versus* distance from the TPPs

	Konakovo TPP				**Cherepetskaya TPP**		
Element	***a***	***b***	R^2	Element	***a***	***b***	R^2
Al	789	-0.17	0.10	**Al**	28200	-0.93	**0.68**
V	44	-0.90	**0.82**	**V**	28	-0.70	**0.62**
Cr	2.1	-0.24	0.17	**Cr**	31	-0.99	**0.75**
Fe	505	-0.16	0.19	**Fe**	4340	-0.59	**0.66**
Co	0.39	-0.20	0.17	**Co**	1.0	-0.35	0.43
Ni	14	-0.71	**0.53**	**Ni**	7.1	-0.38	0.41
As	0.33	-0.38	**0.57**	**As**	1.3	-0.58	**0.53**
Sb	0.12	-0.10	0.06	**Sb**	0.5	-0.59	**0.82**
La	0.87	-0.29	0.34	**La**	0	-0.71	**0.55**
Ce	1.7	-0.17	0.16	**Ce**	31	0.98	**0.75**
Sm	0.19	-0.31	0.38	**Sm**	1.5	-0.76	**0.53**
Tb	0.014	-0.11	0.05	**Tb**	0.33	-0.92	**0.68**
Th	0.13	-0.22	0.26	**Th**	4.3	0.95	**0.66**
U	0.07	-0.26	0.24	**U**	0.97	-0.78	**0.58**

* R^2 coefficient of approximation of power curve

The length of the gradients as the crow flies is 40 km. The spatial distribution is considered similar in all directions from the TPPs since there are no prevailing wind directions in the two examined areas. The local background levels for V (0.73) and Ni (0.28 mg/kg) are reached at a distance of about 30 km from the Konakovo TPP, whereas for Cherepetskaya TPP (Fig. 3) the relevant local background levels are reached at a distance larger than 40 km for such typical coal-fired element-pollutants as U (0.05 mg/kg), Th (0.13 mg/kg), and As (0.17 mg/kg). The same tendency is observed for some rare-earth elements: La (0.7 mg/kg), Ce (0.85 mg/kg), and Sm (0.086 mg/kg) which are also associated with the brown coal-fired TTP.

The intercept with the **y**-axis (parameter ***a***) represents the extrapolated value for moss at the TPP. The slopes of the power curve (parameter ***b***) express the decline of elemental concentration as a function of distance from the TPP. In case of the Konakovo TPP the highest ***b*** values are evident for V and Ni. The slower decline is obvious for such elements as Cr, Fe, Co, As, all rare-earths, Th, and U. On the contrary, for Cherepetskaya TPP the slope decline chracterized by a high negative ***b*** value is rapid for almost all elements listed in the Table. A lower than expected R^2 for Ni (Konakovo TPP) is simply explained by an irregularity in the experimental data (see Fig. 2) caused by another source of Ni in the examined area.

The geographical distributions of some selected elements are shown in Fig. 4.

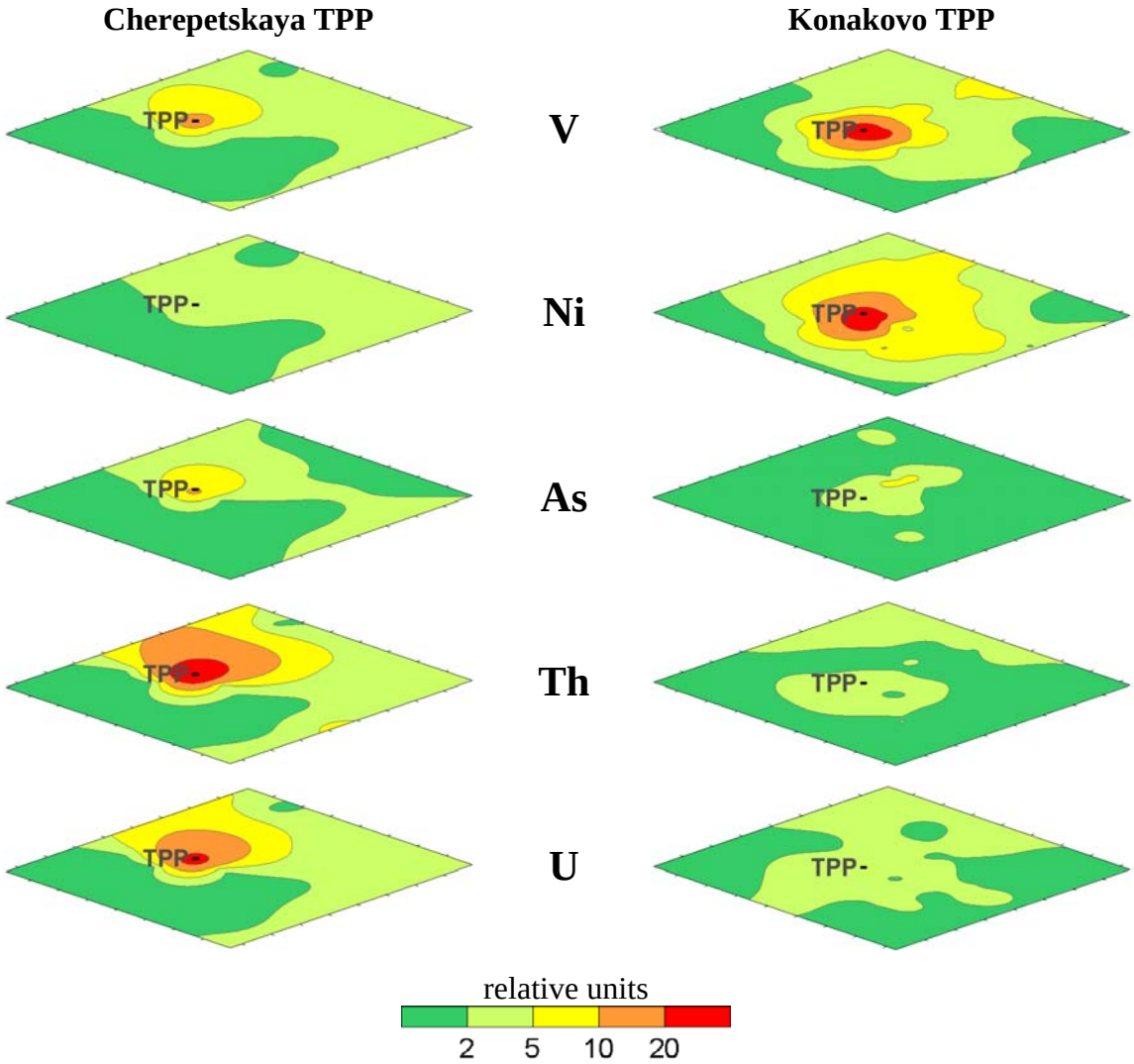

Fig. 4. Geographical distributions of some elements in the studied areas.

Different emission patterns from the two TPPs were found due to the different fuels used for combustion. The results obtained allow one to determine the geographical deposition patterns of heavy metals and other toxic elements. This information should be extremely useful for local administrations and decision-makers responsible for health risk assessment for local residents.

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5. PUBLICATIONS

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8. Kirilov A., Astakhova N., Murashkevich S., Petukhova T., Yudin V. New Generation of the IBR-2 Instrument Control Software in the Windows Environment. Proc. of Germany-JINR User Meeting "Condensed Matter in Physics with Neutrons at IBR-2 Pulsed Reactor", FLNP JINR, Dubna, Russia, June 12-16, 2004, JINR E14-2004-148, Dubna, 2004, pp.118-121.
9. Walter K., Frischbutter A., Scheffzuk Ch., Korobchenko M., Levchanovski F., Nikiforov A., Kirilov A., Astakhova N., Murashkevich S., Petukhova T. EPSILON-MDS: Status quo and Future Development. Proc. of Germany-JINR User Meeting "Condensed Matter in Physics with Neutrons at IBR-2 Pulsed Reactor", FLNP JINR, Dubna, Russia, June 12-16, 2004, JINR E14-2004-148, Dubna, 2004, pp.43-46.

10. Astakhova N., Salamatin I., Schetsov V. Software Complex AS (Automation of Spectrometry). Preprint JINR P13-2003-145. (Submitted in PTE).
11. Kirilov A., Astakhova N., Murashkevich S., Petukhova T., Yudin V.. SONIX+ the New Instrument Control Software at the IBR-2 Reactor. Proc. of the Intern. Workshop “New Opportunities for Better User Group Software”, Villigen PSI, Switzerland, October 18-20, 2004 (in press).
12. Gebauer B., Schulz Ch., Levchanovski F.V, Litvinenko E.I., Nikiforov A.S., Alimov S.S., Wilpert Th. Cross-Fertilization between Spallation Neutron Source and Third Generation Synchrotron Radiation Detectors. AIP Conf. Proceedings, May 12, 2004. Vol.705, pp.1013-1018.
13. Bogdzel A., Bokuchava G., Butenko V., Drozdov V., Zhuravlev V. Kuzmin E., Levchanovski F., Pole A., Prikhodko V., Sirotin A. System for Automation of Experiment on Neutron Fourier Difractometer FSD. Preprint JINR P10-2004-21, Dubna, 2004.
14. Enik T.et at. Microstrip neutron detector with “virtual” cathode. JINR communication (in press).

6. PRIZES

JINR Prizes:

In Experimental Physics Research*:*

Second Prize:

A.I.Frank, I.V.Bondarenko, G.V.Kulin, S.N.Balashov, S.V.Masalovich, V.G.Nosov, A.N. Strepetov, P. Geltenbort, R. Gahler, P. Hoghoj. «Non-stationary influence on the neutron wave at diffraction on the moving grating: prediction, observation and demonstration of possible application»

In Physics Instruments and Methods:

First Prize:

V.D.Ananiev, V.P.Voronkin, L.V.Edunov, V.G.Ermilov, A.F.Zatsepin, Yu.N.Pepelyshev, A.D.Rogov, V.D.Sizarev, I.T.Tretyakov, E.P.Shabalin. «Construction and startup of the new movable reflector MR-3 of heterogeneous type for the reactors IBR-2 and IBR-2M»

In Applied Physics Research*:*

Encouraging Prize:

L.M.Mosulishvili, M.V.Frontasyeva, N.G.Aksenova, A.I.Belokobylskiy, S.F.Gundorina, E.I.Kirkesali, S.S.Pavlov, A.I.Khizanishvili, E.Ya.Tsybakhashvili, V.P.Chinaeva. «Neutron activation analysis in the development of new pharmaceuticals and sorbents on the basis of cyanobacterium Spirulina platensis»

***FLNP Prizes*:**

In Nuclear Physics:

First Prize:

Yu.N.Kopach, Zh.V.Mezentzeva. «Experimental investigations of spontaneous ternary fission of ^{252}Cf».

Second Prize:

A.M.Sukhovoi, V.A.Khitrov «Experimental manifestations of the effect of the assumed breakup of Cooper pairs of nucleons in nuclei of various types».

Third Prize:

S.A.Telezhnikov «Levels of ^{174}Yb populated in averaged capture of resonance neutrons».

In Condensed Matter Physics:

First Prize:

A.M.Balagurov, S.N.Bushmeleva, V.Yu.Pomyakushin. «Magnetic structure of $NdMnO_3$ concordantly doped with Sr and Ru».

Second Prizes:

A.N.Nikitin, T.I.Ivankina, R.N.Vasin. «Applications of neutron scattering in Earth sciences: experimental investigations of rock properties at the IBR-2 reactor».

D.P.Kozlenko, B.N.Savenko. «Effect of high pressures on crystal and magentic structure of manganites $Pr_{1-x}Sr_xMnO_3(x=0,5-0,56)$».

Third Prize:

M.A.Kiselev «Study of cryoprotective properties of dimethylsulfoxide by real-time diffraction».

In Applied and Methodical Physics:

First Prize:

A.S.Kirilov, N.V.Astakhova, S.M.Murashkevich, T.B.Petukhova, V.E.Yudin «Sonix and Sonix+ control software packages for spectrometers at the IBR-2 reactor».

I.M.Frank Stipend:

In Nuclear Physics:

E.V.Ermakova

In Condensed Matter Physics:

V.I.Bodnarchuk

In Methodical Investigations:

V.E.Yudin

7. SEMINARS

Date	Authors	Title
25.03.04	E.P.Shabalin (FLNP JINR) A.M.Balagurov (FLNP JINR)	History of development of movable reflectors and cold moderators at the IBR-2 reactor Neutron diffraction at the IBR-2 reactor
8.04.04	V.B.Priezzhev (BLTP JINR)	Non-stationary solutions for non-equilibrium processes (kinetics of fluxes of interacting particles)
10.06.04	V.V.Nietz (FLNP JINR)	Time-of-flight method and neutron investigations of condensed matter with a pulsed magnetic field (Doctor Thesis)
9.11.04		Seminar dedicated to the 80-th anniversary of L.B. Pikelner
24.12.04		«Decembrists in the scientific life of FLNP», dedicated to the 70-th anniversary of V.V. Golikov, Zh.A. Kozlov, V.I. Luschikov

8.1. STRUCTURE OF LABORATORY AND SCIENTIFIC DEPARTMENTS

Directorate:
Director:
A.V.Belushkin
Deputy Directors:
N.Popa
V.N.Shvetsov
Scientific Secretary:
V.A.Khitrov

Reactor and Technical Departments
Chief engineer: V.D.Ananiev
IBR-2 reactor
Chief engineer: A.V.Vinogradov
Department of IREN
Head: V.G.Pyataev
IBR-30 booster + LUE-40 Group
Head: S.A.Kvasnikov
Mechanical maintenance division
Head: A.A.Belyakov
Electrical engineering department
Head: V.P.Popov
Design bureau
Head: A.A.Kustov
Experimental workshops
Head: A.N.Kuznetsov

Scientific Departments and Sectors
Condensed matter department
Head: V.L.Aksenov
Nuclear physics department
Head: Yu.N.Kopatch
Department of IBR-2 spectrometers complex
Head: A.V.Belushkin
Nuclear Safety and applied research sector
Head: E.P.Shabalin

Administrative Services
Deputy Director: S.V.Kozenkov
Secretariat
Finances
Personnel

Scientific Secretary Group
Translation
Graphics
Photography
Artwork

CONDENSED MATTER DEPARTMENT

Sub-Division	Title	Head
Diffraction sector. Head: A.M.Balagurov		
Group No.1	HRFD	V.Yu.Pomjakushin
Group No.2	DN-2	A.I.Beskrovnyi
Group No.3	DN-12	B.N.Savenko
Group No.4	NSVR	A.N.Nikitin
Group No.5	SKAT	Ch.Scheffzük
Small-angle neutron scattering group. Head: V.I.Gordeliy		
Neutron optics sector. Head: V.L.Aksenov		
Group No.1	REMUR	Yu.V.Nikitenko
Group No.2	REFLEX	V.I.Bodnarchuk
Group No.3	BIOPHYSICS INVESTIGATIONS	I.N.Serdyuk
Inelastic scattering group. Head: I.Natkaniec		

NUCLEAR PHYSICS DEPARTMENT

Sub-Division	Title	Head
Sector 1. Correlation γ-spectroscopy and development of experimental installations. Head: N.A.Gundorin		
Sector 2. Polarized neutrons and nuclei. Head: Yu.D.Mareev		
Group No.1	Polarized nuclear targets	Yu.D.Mareev
Group No.2	Thermal polarized neutrons	M.I.Tsulaya
Sector 3. Neutron activation analysis. Head: M.V.Frontasyeva		
Group No.1	Analytical	M.V.Frontasyeva
Group No.2	Experimental	S.S.Pavlov
Group No.2	**Neutron spectroscopy**	**Yu.N.Kopatch**
Group No.3	**Nuclear fission**	**Sh.S.Zeinalov**
Group No.5	**Proton and α-decay**	**Yu.M.Gledenov**
Group No.6	**Properties of γ-quanta**	**A.M.Sukhovoy**
Group No.7	**Neutron structure**	**V.G.Nikolenko**
Group No.8	**Ultra-cold neutrons**	**A.V.Strelkov**
Group No.9	**Neutron optics**	**A.I.Frank**
Group No.11	**Theory**	**V.K.Ignatovich**
Group No.12	**Electrostatic generator-5**	**I.A.Chepurchenko**

DEPARTMENT OF IBR-2 SPECTROMETERS COMPLEX

Sub-Division	Title	Head
Group No.1	Scintillation detectors	E.S.Kuzmin
Group No.2	Gaseous detectors	Ts.Panteleev
Sector No.1	**Electronics**	**V.I.Prikhodko**
Group No.1	Analog electronics	A.A.Bogdzel
Group No.2	Digital electronics	V.F.Levchanovsky
Group No.3	Software	A.S.Kirilov
Group No.4	Local network	G.A.Sukhomlinov
Group No.5	Technology	A.B.Melnichuk
Sector No.2	**Spectrometers**	**A.P.Sirotin**
Group No.1	Development of spectrometer elements	A.P.Sirotin
Group No.2	Sample environment	A.N.Chernikov

8.2. USER POLICY

In 2004 has been elaborated a new program for the users of the IBR-2 spectrometers. The program has been conceived to balance reasonably between the staff needs to accomplish the maintenance work, contracts and long-term projects and the availability to put the IBR-2 facilities in an open system of international collaboration. Every year the reactor will operate for 8 cycles of 2 weeks. The reactor run time is divided as follows: 36% for staff, 53% for users with regular access, 11% for users with fast access.

The access of users to experiments is permitted only on application basis. For regular applications there is a deadline for submission, 20 September, and a review process for time allocation. The fast access applications have not deadline, nor a review process, but the permission for experiment is granted only in exceptional cases. All applications are submitted only by the electronic mail.

The review process for the regular application has three stages. In the first stage the instrument scientists select the feasible proposals and send them to the referees by the electronic mail. In the second stage every referee, independently, sets up a list of proposals ordered according to his opinion. The third stage is the meeting of the experts that decide by consensus the final list of accepted experiments. The schedule for experiments is made according to the final list by the head of the Condensed Matter Department together with the instrument scientists.

The review process is carried out by four commissions, every one composed from three independent experts. Four fields of expertise are covered: diffraction, inelastic scattering, neutron optics and small angle scattering.

All information connected to the users' policy can be found on the laboratory website.

8.3. MEETINGS AND CONFERENCES

In 2004, FLNP organized the following meetings:

1.	Seminar dedicated to the 25-th Anniversary of the IBR-2 Reactor	March 25	Dubna
2.	SAD International Workshop	January 26-27	Dubna
3.	XII International Seminar on Interaction of Neutrons with Nuclei (ISINN-12)	May 26-29	Dubna
4.	III JINR – Germany User Meeting «Condensed Matter Physics with Neutrons at the IBR-2 Pulsed Reactor»	June 12-16	Dubna

In 2005, FLNP will organize the following meetings:

1.	XIII International Seminar on Interaction of Neutrons with Nuclei (ISINN-13)	May 25-28	Dubna
2.	Workshop on Investigations at the IBR-2 Pulsed Reactor	June 15-17	Dubna

8.4. COOPERATION

List of Visitors from Non-Member States of JINR in 2004

Name	Organization	Country	Dates
K.Walther	GeoFRZ, Potsdam	Germany	19.01-30.01
A.Frischbutter	GeoFRZ, Potsdam	Germany	23.01-30.01
J.-J.Fundenberger	University of Metz	France	17.03-19.03
F.Wagner	University of Metz	France	17.03-19.03
H.Scheben	Univ., Freiburg	Germany	17.03-19.03
H.-J.Lauter	ILL, Grenoble	France	17.04-21.04
K.Walther	GeoFRZ, Potsdam	Germany	19.04-30.04
A.Frischbutter	GeoFRZ, Potsdam	Germany	19.04-28.04
J.Stuller	IAEA, Vienna	Austria	26.04-27.04
B.Crawford	Physics College, Gettysburg	USA	20.05-29.05
E.Steinnes	Univ., Tondheim	Norwey	02.06-05.06
R.E.Jervis	Univ. of Toronto	Canada	08.06-12.06.
M.-T.Rekveldt	TU, Delft	The Netherlands	09.06-15.06.
E.Osawa	NanoCarbon Research Inst.Ltd., Chiba	Japan	10.06-12.06
K.Noak	FZ, Rossendorf	Germany	21.06-27.06
Mai Khan Tran	High Tech Company, Reston	USA	21.06-05.07
Duong Lien Bach	High Tech Company, Reston	USA	21.06-05.07
K.Walther	GeoFRZ, Potsdam	Germany	13.07-23.07
L.Rosta	KFKI, RIPNP, Budapest	Hungary	20.07-25.07
M. Loevenhaupt	Univ., Dresden	Germany	01.08-05.08
M.V.Simkin	Univ. of California, Los Angeles	USA	04.08-06.08
K.Ullemeyer	Univ., Freiburg	Germany	06.09-26.09
A.A.Podlesnyak	PSI, Villigen	Switzerland	17.09-20.09
S.Kennedy	Bragg Institute	Australia	21.09-22.09
J.Zaccai	CNRS, Grenoble	France	01.10-30.10
O.Steinswoll	Institute for Energy Technology, Kjeller	Norway	18.10-02.11
E.Raitman	IPE, Riga	Latvia	21.10-21.10
J.-S.Teixeira	LLB , Saclay	France	27.10-04.11
J.Wummel	GeoFRZ, Potsdam	Germany	08.11-16.11
F.Wobbe	Univ., Freiburg	Germany	08.11-12.12
G.Pepy	LLB, Saclay	France	11.11-18.11
K.Walther	GeoFRZ, Potsdam	Germany	11.11-24.11
V.Lauter	ILL, Grenoble	France	14.11-23.11
H.-J.Lauter	ILL, Grenoble	France	17.11-23.11
P.M.Bokov	CEA, Saclay	France	16.11-17.11
K.Ullemeyer	Univ., Freiburg	Germany	01.12-12.12
P.Geltenbort	ILL, Grenoble	France	03.12-05.12
K.Walther	GeoFRZ, Potsdam	Germany	07.12-17.12
L.Almasy	KFKI RIPNP, Budapest	Hungary	16.12-22.12
N.Szekely	KFKI RIPNP, Budapest	Hungary	16.12-22.12

8.5. EDUCATION

The objective of the FLNP educational program is the training of specialists in the field of neutron methods for condensed matter and nuclear physics research. The students of neutron diffraction department of MSU and the students of the MSU Interfaculty Center «Structure of Matter and New Materials» carry out their diploma works in FLNP. At the Center the students from the Chemical Faculty of MSU, Higher College of Materials Sciences of MSU, Tula State University, Tver State University and other universities of Russia and JINR member-states do the course.

In 2004 two schools and two practices on condensed matter with neutrons were organized.

In February (2^{nd} – 6^{th}) the Winter School for the students of neutron diffraction division of Physical Department of MSU took place.

From the 10^{th} of February to the 5^{th} of March the practice for the students of New Material Department of MSU was organized.

From the 28^{th} of June to the 2^{nd} of July the Summer School for the students of neutron diffraction department of MSU was held.

In September there were the practices for students of Technical University – "Ural Polytechnical Institute (UPI)", for Polish students from Poznan, for Romanian students and students from Kostroma and Kiev State Universities.

8.6. PERSONNEL

Distribution of the Personnel per Department as of 01.01.2004

Theme	Departments	Main staff
-1036-	Nuclear Physics Department	65
-1031-	Condensed Matter Physics Department	42
-1052-	IBR-2 Spectrometers Complex Department	41
-0993-	IREN Department	12
-0851-	IBR-2 Department	46
	Mechanical and Technical Department	50
	Electric and Technical Department	32
	Central Experimental Workshops	36
	Nuclear Safety Sector	12
	Design Bureau	7,5
	FLNP infrastructure:	
	Directorate	8
	Services and Management Department	23
	Scientific Secretary Group	7
	Supplies Group	3.5
Total		**385**

Personnel of the Directorate as of 01.01.2004

Country	People
Bulgaria	1
China	1
Germany	2
Georgia	2
Kazakhstan	1
KPDR	5
Poland	3
Romania	6
Russia	25
Slovakia	2
Ukraine	5
TOTAL	**53**

8.7. FINANCE

Financing of the FLNP Scientific Research Plan in 2004 (th. USD)

No.	Theme	Financing plan, $ th.	Expenditures for 12 months, $ th.	In % of FLNP budget
I	**Condensed matter physics**	**4011.9**	**3214.0**	**80.0**
	-1031-	2291.6	1897.5	82.8
	-0851-	936.8	803.7	85.8
	-1052-	783.5	512.8	65.5
II	**Neutron nuclear physics**	**1046.1**	**1061.8**	**101.5**
	-1036-	694.9	722.9	104.0
	-0993-	351.2	338.9	96.5
III	**Elementary particle physics**			
	-1007-	**6.0**	**27.5**	**458.0**
IV	**Relativistic nuclear physics**			
	-1008-	**40.6**	**13.9**	**34.2**
V	**TOTAL:**	**5104.6**	**4317.2**	**84.6**

12 International Seminar on Interaction of Neutrons with Nuclei
ISINN 12

N.V. Kornilov, A.Yu. Muzychka,
G.G. Bunatian, V.G. Nikolenko,
S.S. Parzhitskiy during
The discussion

S. Pospišil, Yu.A. Aleksandrov

At the barbecue

Discussion in the “warm company”:
V.N. Shvetsov, A.V. Strelkov,
V.I. Furman, Yu.N. Kopach,
M.Daum

Seminar dedicated to the 80-th anniversary of L.B. Pikelner

Story by the jubilarian about his scientific work before the creation of JINR and FLNP

A.M. Balagurov, E.Ya. Pikelner, V.I. Furman, D.N. Bell, T.L. Pikelner, L.B. Pikelner

FLNP Director A.V. Belushkin and the jubilarian

All Heads of the FLNP Nuclear Physics Department in chronological order (left to right): V.I. Luschikov, L.B. Pikelner, V.I. Furman, V.N. Shvetsov, Yu.N. Kopach

Preparation of new experiment

Vacuum over-reactor channel to investigate the direct measurement of the nn-scattering length at the pulsed reactor JAGUAR (Snezhinsk)

Construction of the IREN source

New storage building 117/6 for displacement of activated elements of IBR-30 reactor

The linac LUE-200 grid and modulator