1. SCIENTIFIC RESEARCH

1.1. CONDENSED MATTER PHYSICS

Organization of research work and instrument development. In 2002 under theme 1031, neutron scattering investigations in condensed matter physics were mainly conducted at the IBR-2 reactor. In addition, physicists of the FLNP Scientific Department of neutron investigations of condensed matter working within the framework of theme 1031 carried out a number of experiments in neutron laboratories of Europe by the accepted proposals. During the reported year IBR-2 operated for eight working sessions. The beam time for experiments at the reactor spectrometers was distributed in accordance with the recommendations of experts on the submitted proposals and existing long-term agreements.

In 2002, scientific investigations were carried out on 10 spectrometers: HRFD, DN-2, DN-12, SKAT, YuMO, EPSILON, REFLEX-P, KDSOG, NERA, and DIN. A large volume of methodical works was performed on the spectrometers FSD, SPN, EPSILON, and REFLEX-P. On the neutron Fourier diffractometer FSD intended to study internal stresses in materials and engineering products, work on the detector system continued. In particular, in October two new elements of ±90°-detectors based on ZnS(Ag)-scintillators of modernized configuration with an increased solid angle, were installed. During the year on SPN a radical modernization was carried out as a result of which the installation of a new head part of the spectrometer was completed, the multichannel neutron polarizer intended for small-angle investigations was put into operation (its polarization efficiency exceeded 90% in a wide interval of wavelengths), and the multichannel efficient focal analyzer of polarization was commissioned. On EPSILON, nine new detectors with collimators were installed, thus, the number of detectors was increased to 36. On REFLEX-P, the neutron-optical system was assembled anew, resulting in a 4-times enhancement of polarized beam intensity. In addition, methodical work on the improvement of parameters, experimental conditions and primary data processing continued on all the IBR-2 spectrometers.

Scientific results. Diffraction. In 2002, as the investigations of the $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ (LPCM-*y*) compound continued, a series of neutron diffraction experiments (with HRFD, DN-12 and DMC on SINQ source) to obtain information on the magnetic phase diagram of the compounds with the predominance of ^{18}O isotope (up to 75%) were carried out. Their main result is that the phase diagrams of LPCM-*y*/^{16}O and LPCM-*y*/^{18}O are qualitatively identical (**Fig.1**). This gives grounds to believe that the giant isotope effect in electroresistance, observed earlier for the LPCM compound with y=0.75, is a manifestation of a transition to another phase state (for more details see Experimental Reports).

The crystal and magnetic structures of the new layered complex manganese oxide Sr_2MnGaO_{5+x} with an intermediate content of oxygen x=0.13 and 0.41 (between the limiting values x=0 and 0.5) were investigated. As was demonstrated earlier in the limiting cases the magnetic structures differ significantly and correspond to antiferromagnetic (AFM) *G*- and *C*-types for x=0 and 0.5, respectively. It turned out that while the composition with x=0.13, as the temperature decreases (T_N≈200 K), undergoes a transition to a homogeneous antiferromagnetic state of *G*-type (i.e. its behavior is the same as of the composition with x=0), in the composition with x=0.41 magnetic phases of both *G*- (T_N≈140 K) and *C*- (T_N≈110 K) types with approximately equal concentrations appear (**Fig.2**). The unusual fact is the lack of evidence of any structural differences in the two arising magnetic phases.

On the DN-12 spectrometer, a lot of experiments to study the behavior of both the atomic and magnetic structures of crystals at high pressures were conducted. For example, the crystal structure of mercury chalcogenides $HgSe_{0.7}S_{0.3}$ and $HgTe_{0.85}S_{0.15}$ in the pressure range up to 8 GPa was investigated. On the basis of the obtained structural data the phenomenological model of a structural phase transition from a cubic blende structure to hexagonal cinnabar structure occurring in these compounds, was suggested.

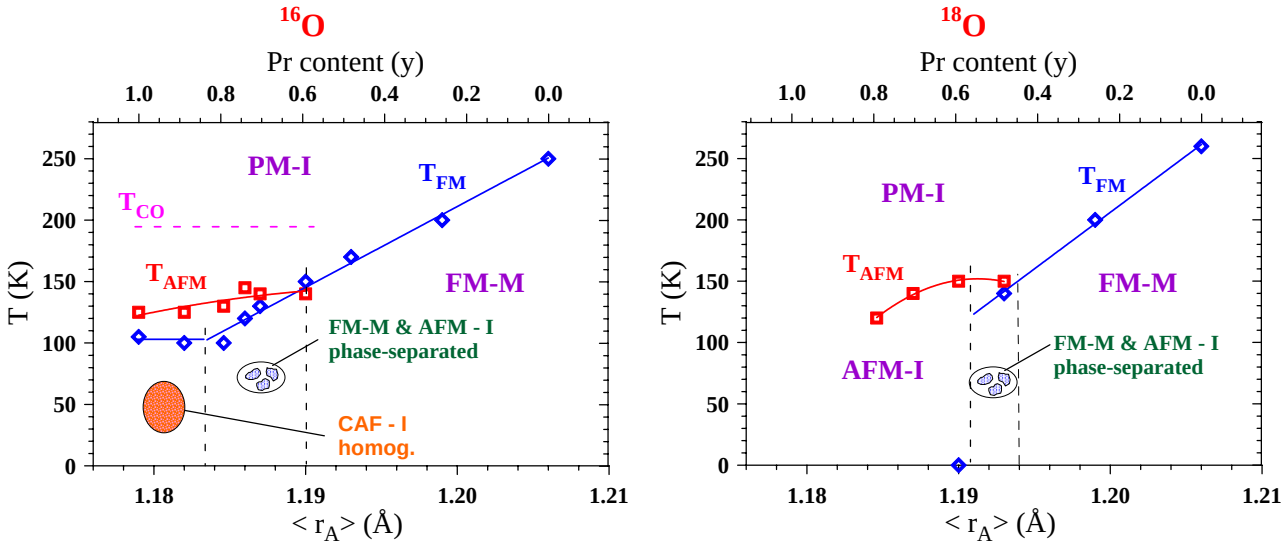

Fig.1. *Magnetic phase diagrams for the* $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ *compositions containing oxygen isotopes* ^{16}O *(left) and* ^{18}O *(right).*

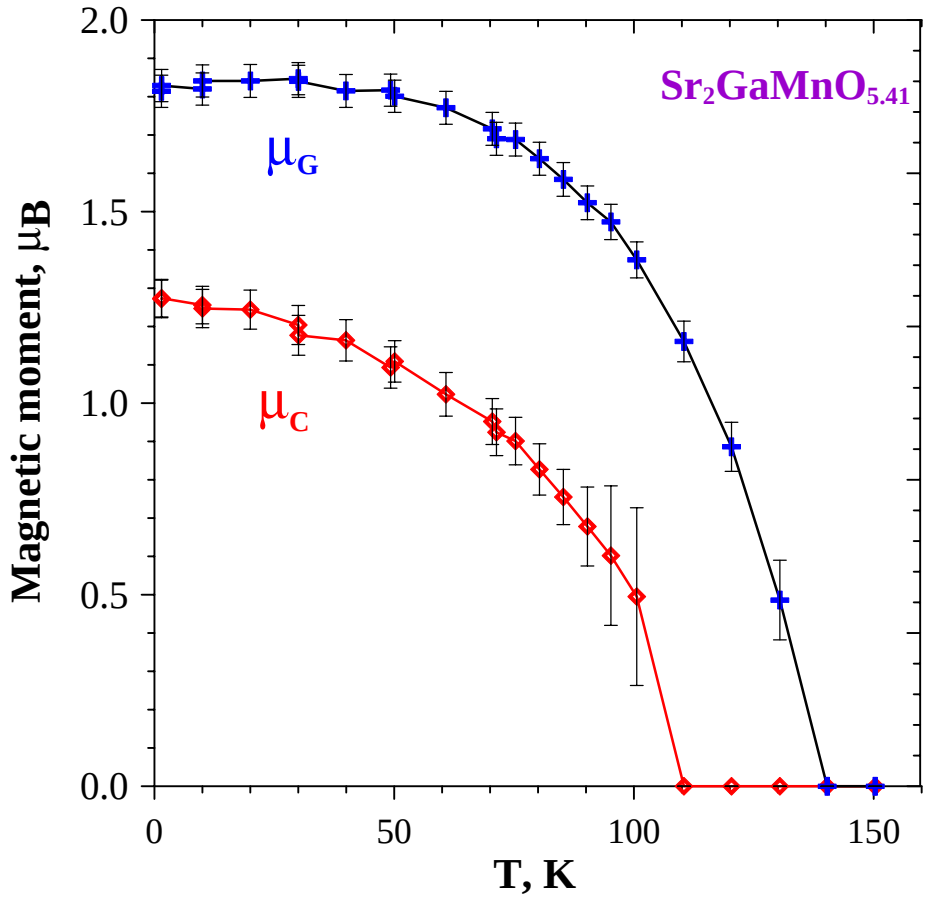

Fig 2*. Dependence of the value of magnetic moments in* $Sr_2MnGaO_{5.41}$ *on temperature. At* $T \approx 140$ *and 110 K there occur two sequential magnetic phase transitions with the formation of the G- and C-type antiferromagnetic phases, i. e. magnetic phase separation develops.*

The crystal and magnetic structures of manganites $Pr_{0.7}Ca_{0.3}Mn_{1-y}Fe_yO_3$ (y=0, 0.1) and $Pr_{0.8}Na_{0.2}MnO_3$ with the CMR effect were investigated at pressures up to 4.5 GPa and in the temperature interval from 16 to 300 K with the DN-12 spectrometer. For the first time it was found that in these compounds, which have significantly different magnetic structures at a normal pressure

($Pr_{0.7}Ca_{0.3}MnO_3$ and $Pr_{0.8}Na_{0.2}MnO_3$ have the AFM structure of pseudo-*CE* type, while $Pr_{0.7}Ca_{0.3}Mn_{0.9}Fe_{0.1}O_3$ is ferromagnetic), stabilization of the AFM state of type *A* with characteristic propagation vector **q**=(010) takes place at high pressures and low temperatures (for more details see Experimental Reports).

The effect of quasihydrostatic pressure up to 4 GPa and hydrostatic pressure up to 2.5 GPa on Fe_2O_3 was studied. It was revealed that in quasihydrostatic conditions even at pressure P~2 GPa a spin-reorientation phase transition occurs, resulting in a change of the angle of Fe magnetic moments in respect to rhombohedral axis (111) of the crystal. At the same time, in hydrostatic conditions up to pressure 2.5 GPa the reorientation of magnetic moments was not observed.

On DN-2, $Pb_{0.8}Sn_{0.2}Te$ monocrystals in which anomalies in temperature dependence of some macroscopic properties had been earlier detected, were studied. The diffraction experiments verified the hypothesis about multiple phase transformations in this compound. The situation in $Pb_{0.8}Sn_{0.2}Te$ appears to be analogous to that observed in the narrow-gap semiconductor InSe for which the analysis of kinetic, galvanomagnetic and thermoelectric phenomena testifies the existence of structural Peierls phase transitions. Moreover, the temperature dependence of specific resistance investigated for InSe suggests the instability of structure and presence of some phase transformations. To clear up the situation it is proposed to carry out structural investigations of InSe on mono-and polycrystalline samples.

Small-angle neutron scattering. Within the framework of studies of cluster state of fullerenes in solutions the experiments on small-angle neutron scattering from the solution of C_{60} in carbon disulfide (C_{60}/CS_2) and the colloidal solution of C_{60} in water (C_{60}FWS) were performed. For the system C_{60}/CS_2 it was shown that the formation of small clusters with the mean aggregation number of about four takes place in solution. The aggregation number does not depend on the temperature ($15 \div 30^oC$) and concentration ($4 \div 8$ mg/ml). These results cast doubt on the use of the drop model to describe the cluster structure in solution. In the case of C_{60}FWS large polydispersity over a wide range of sizes up to 50 nm was revealed. The contrast variation based on different mixtures of light and heavy water points to the presence of a component in the aggregates, which is different from fullerenes. This component is assumed to be responsible for stabilization of the dispersions. A number of hypotheses about its origin, in particular, the formation of a specific hydration shell around fullerenes, are being discussed (for more details see Experimental Reports).

The conformation of the elongation factor eFF1A from mammal cells (rabbit) in solutions was investigated by means of small-angle neutron scattering and scanning microcalorimetry. It was found that in contrast to a bacterial analogue the protein has no fixed structure in solution. This follows from the fact that the radius of gyration, 5.2 nm, determined from the small-angle scattering curves is considerably greater than that of the prokaryotic eEF1A, while the specific heat of denaturation of the studied eEF1A, 4 cal/g, obtained by the scanning microcalorimetry is significantly lower than 7 cal/g for the prokaryotic eEF1A calculated for the same denaturation temperature. The small-angle neutron scattering data suggest that the studied eEF1A becomes more compact when forming a complex with the diacyl-tRNA.

Polarized neutrons and neutron optics. The reflectometry was applied to study the interface formation during the synthesis of multilayers from the P(dS-b-nBMA) copolymers composed of blocks with different molecular weight. It was found that the numerous peculiarities observed in the off-specular neutron scattering spectra are connected with the presence of islands or pores randomly distributed on the film surfaces, as well as with the formation of complex interphase boundaries.

Within the framework of investigations of multilayer magnetic structures the reflectometry experiments on the MgO (001) / $[Fe(x\ ML) / V(y\ ML)]_N$ / Pd structures were carried out. The magnetization profile and distribution of Fe and V atoms at interfaces were obtained. Nuclear and magnetic potentials drop faster and grow more rapidly upon passing the interface in a direction

from vanadium to Fe than in a direction from Fe to vanadium. This fact is determined by the asymmetry in the interpenetration of Fe and vanadium atoms.

On the REFLEX-P spectrometer, the high-precision experiment to search for the surface magnetic excitations in magnetic thin film structures was continued. A full set of experimental data has been collected, and at the present time the creation of a mathematical model to treat the obtained results is in progress.

Inelastic neutron scattering. On the NERA spectrometer, the structural phase transitions and dynamics of solid mesitylene, as well as the influence of concentration and temperature on the dynamics of ammonium groups and phase transitions in mixed crystals $Rb_{1-x}(NH_4)_xBr$, were investigated. Mesitylene known as an organic solvent with a comparatively low freezing point of 227 K holds much promise for cold neutron sources. The results of simultaneous measurements of both the diffraction and inelastic neutron scattering demonstrated that the phase composition of solid mesitylene depends on the cooling rate, i.e. mesitylene is an interesting example of a relatively simple molecular crystal which exists at low temperatures in various structural modifications with significantly different dynamic characteristics (**Fig.3**). In the future this will make it possible to study the packing effect on the lattice dynamics and rotation dynamics of methyl groups (for more details see Experimental Reports).

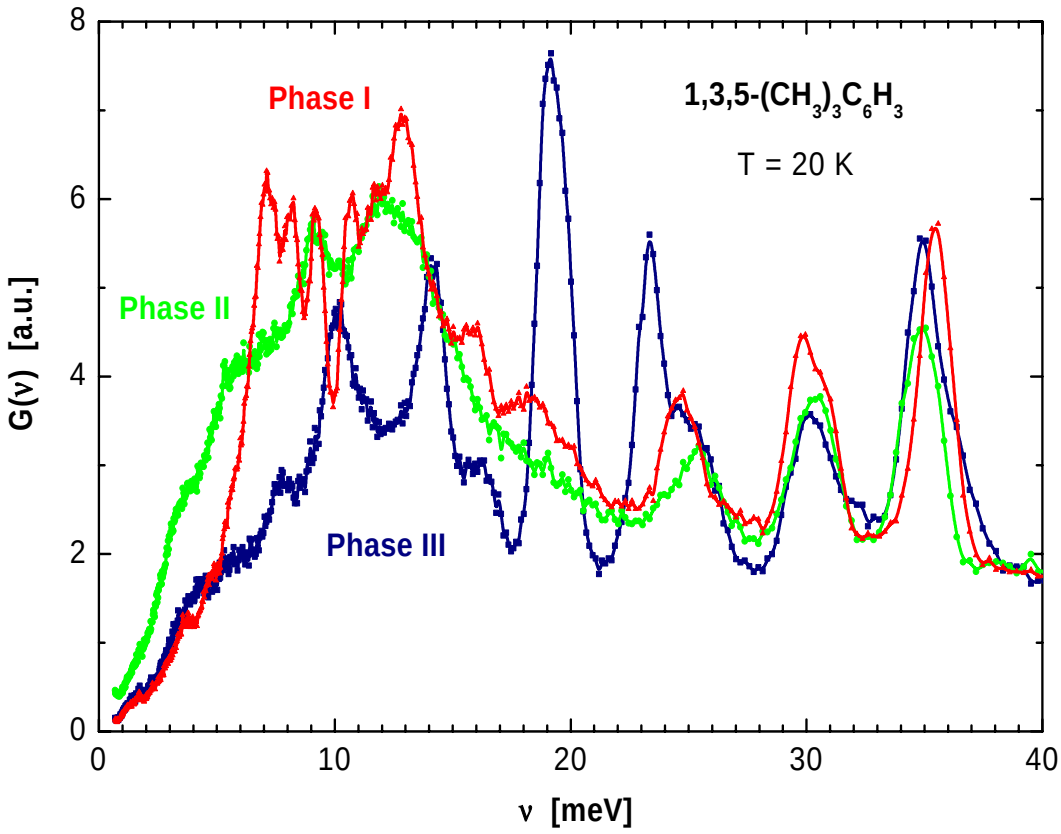

Fig.3. *Phonon state density in different structural phases of mesitylene.*

The investigations of the crystalline electric field (CEF) effects in $RAgSb_2$, where R=Ce, Tm, Er and Ho, were carried out by means of inelastic neutron scattering. The CEF parameters, as well as the level schemes and wave functions were determined. The temperature dependence of magnetic susceptibility calculated for different crystallographic directions using the CEF parameters agrees well with the experimental results for monocrystals. The analysis shows that magnetocrystalline anisotropy in these compounds is determined mainly by CEF.

Applied research. The diffraction study of textures of amphibolites and gneisses from the section of the super deep borehole SG-3 in Kola Peninsula and their analogues from the surface, continued. The modelling of the elastic wave speed distribution in the studied samples was conducted using the quantitative information on the texture and data on elastic modules of rock-forming minerals. The analysis of the obtained data will allow us to find out the contribution of the oriented mineral components into the total elastic anisotropy of rocks. This is necessary to establish regularities between texture peculiarities and deformation mechanisms, as well as metamorphic processes responsible for the texture formation in the process of evolution of lithosphere.

Complex application of neutronographic texture analysis and ultrasonic spatial sounding of spherical samples at various high pressures made it possible to provide a physical explanation to different character of change in anisotropy of mantle olivinite properties and to establish the fact of reduction in anisotropy factor with an increase in pressure for olivine xenolites.

Shock deformation of samples consisting of sandstone and olivine was investigated. For this purpose strain values for untextured multiphase sandstone, containing quartz, various kinds of feldspar and mica were measured. The sample was shock deformed to model conditions of strong impact. The deformation was scanned across the interface between dunite (olivine) and quartzite (quartz). The data obtained with the help of time of flight neutron diffraction were analyzed together with the results of research performed using X-ray synchrotron radiation and microstructural measurements. The results show that residual strains differ widely depending on a characteristic combination of texture, peculiarities of applied deformation and microstructural features of rocks. The grain size of scattering crystals was estimated by analyzing peak profiles (synchrotron radiation diffraction) on each side of the phase interface.

To explain the swelling mechanism in graphite blocks irradiated by neutron fluxes, a number of in-situ experiments to study changes in anisotropy in the samples of reactor graphite under the action of compression stresses, were carried out. Investigations were performed both in elastic and plastic deformation regions. It was found that the graphite crystal lattice remains unchanged until stresses are close to the breaking stress value. It is possible that this unusual result can be connected with the initial porosity of the samples, i.e. the action of compression stresses reduces to the collapse of pores without significant elastic deformation of the crystal lattice. The obtained data will be verified on the graphite samples cut out from different places and variously arranged locations in the reactor block.

On the DN-2 diffractometer, the ordering phenomenon in NiCr alloy, which is a constructional material, was studied. A number of NiCr-based compounds doped with Mo, Si and S were investigated. Plates annealed at temperatures of 300, 350, 400 and 450°C were used as samples. Only in one (alloy 32XHM annealed at T=450°C) of 32 studied samples superstructure diffraction peaks indicative of the ordering of Ni and Cr atoms were detected. It was found that in this sample the superstructure Ni_2Cr is formed. Upon ordering, chrome and nickel atoms are arranged on planes (110) of initial cubic cells (space group Fm3m, a=3.62 Å) so that one layer of chrome is followed by two layers of nickel. The unit cell of this lattice is orthorhombic (Pnnm) with a =7.653 (1), b =2.560 (1) and c = 3.631 (1) Å. The ordering proceeds in the whole bulk of the sample.