1.1. CONDENSED MATTER PHYSICS

Late in 1998 the Condensed Matter Physics Department (CMPD) was reorganized with the aim of concentrating effort on scientific activity itself. Diffraction, small angle scattering, inelastic scattering, and neutron optics continued to be the basic neutronographic methods used by CMPD members to carry out experiments with the IBR-2 spectrometers. During the year there were eight reactor cycles at a mean power of 1.5 MW. As in the past few years the beam time was distributed on experts' recommendation based on submitted proposals and long-term agreements for cooperation. The 1999 list of spectrometers operating in the user mode included 10 instruments: HRFD, DN-2, DN-12, SKAT, YuMO, SPN, REFLEX-P, KDSOG, NERA, and DIN. Several experiments were conducted with the spectrometer TEST in channel 6B.

By spring 1999 laying of a neutron-guide for carrying out diffraction measurements of residual stresses in large-volume products on the new Fourier diffractometer FSD had completed. In May 1999 neutron beam profiles were measured at the exist of the mirror neutron guide and at the sample position. The obtained absolute fluxes appeared to be close to expected. In 1999, a biological shielding was laid and a Fourier chopper manufactured using an improved technology was installed on FSD. In April 2000, the first stage of the FSD detector system and the FSD correlation electronics will start operation. After that regular measurements with FSD will begin.

A smooth transition of the detecting and control electronics of the neutron spectrometers to VME standard continued. During the year the new electronics of another two spectrometers, FHRD and YuMO, was commissioned. It allows essential automation of the experiment, including remote control. In particular, the new software for YuMO is a multiwindow system that controls motors, temperature, and experimental data acquisition.

1. Methodological. In the operating Fourier diffractometer HRFD (IBR-2 channel 5) the rotor and stator of the Fourier chopper were replaced by new ones analogous to those installed in FSD. Contrast measurements of the new system showed that the contrast had grown to a value of 20 (about 3 times). This improves considerably the quality of the registered diffraction spectra. In the high pressure diffractometer DN-12 a closed-cycle refrigerator-based cryostat is put into operation to conduct measurements under simultaneous action of low temperatures down to 12 K and high pressures up to 7 Gpa. The first scientific experiments were carried out.

On the polarized neutron reflectormeter REFLEX-P test experiments of the inelastic scattering mode were performed. The mode is designed to carry out investigations of the inelastic interaction of neutrons with surface excitations in thin films. The spectrometry of the scattered neutrons is conducted in the direct geometry with a fast chopper in front of the sample for the monochromatization of the incident beam (Dl/l=0.04/l). Experiments to investigate a Ni/Ti thin film and a FeCo/TiZr supermirror showed that this direction of the physics of thin films is a promising field of research with the reflectometer REFLEX-P.

For the spectrometer DIN-2PI, assembling of control systems for the thermostat TS3000 which will make it possible to investigate materials at temperatures to 3000 K started.

In the reported year most important was the testing of a cryogenic methane moderator (CM) which was installed in October 1999 on the side of beams 4 (YuMO), 5 (DN-2), and 6 (HRFD). During the followed three reactor cycles information about the CM parameters was obtained. **Figure 1** illustrates the obtained spectra of scattering on vanadium for three different states of the moderator: with methane at 30 K or 60 K, with an empty chamber and a water premoderator, T=300 K. In addition to the shifting of the maximum in the spectrum in the direction of larger wavelengths with decreasing temperature, it is characteristic of the CM spectrum to have a strong eating-away in the region of the Be-boundary (l=3.96, 3.58, and 3.46 E) due to the moderator design. In the warm state, i.e. without methane, CM is inferior to a standard grooved moderator (GM) especially at wavelengths lower than 4 E where the score is 1 to 3. In the cold state CM gives a considerable gain in comparison with GM: at T=70 K starting from l=2 E and at T=30 K starting from l=3 E (**fig. 2**).

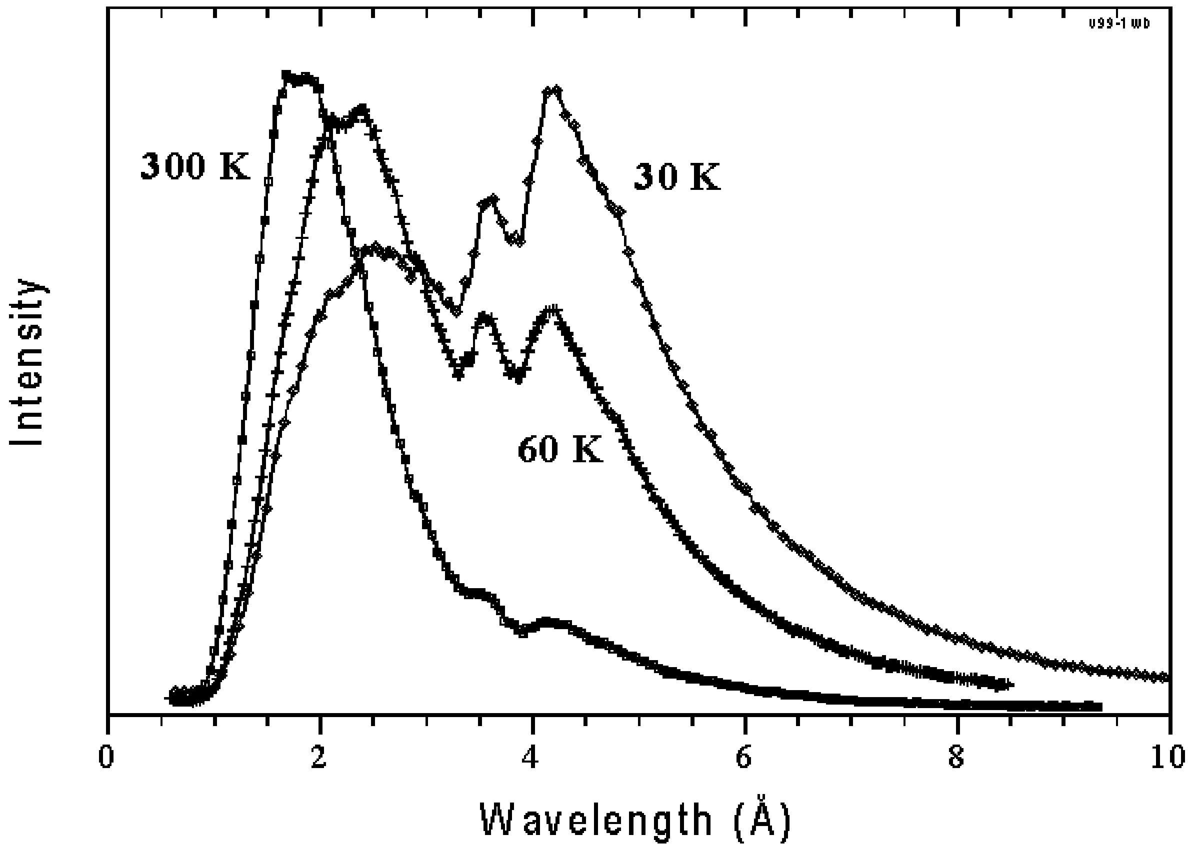


Fig.1. *The spectra registered with HRFD using the detector D1 for three different states of the moderator: T=60 K, 30 K, and 300 K (empty chamber, water premoderator).*

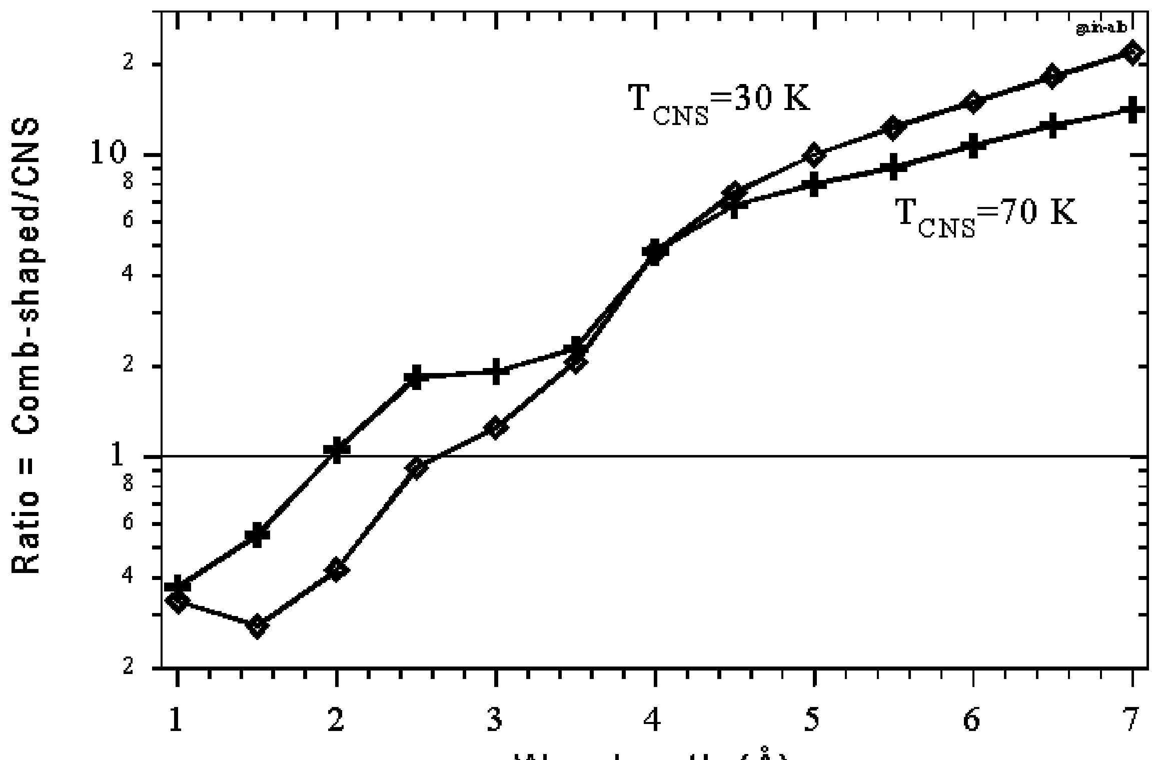


Fig.2. *The coefficient of gain (loss) at transition from a grooved moderator (300 K) to CM (30 K or 70 K) as determined from scattering on Al_2O_3 or V.*

The most detail data on CNS parameters were obtained with HRFD. Their analysis prompted the following conclusions.

- Problems solved with the diffractometer HRFD or DN-2 can be **optimally divided** between experiments with the moderator in the warm or cold mode.
- **The cold moderator makes it possible** to study effectively low-symmetry structures with a unit cell volume of ~500 E as well as magnetic and long-period structures using HRFD.
- The moderator temperature 70 K **is optimal** for the solution of the enumerated problems.

As to small angle neutron scattering investigations of macromolecular systems in solutions (e.g., ribosomes) the cold moderator will also make it possible to start experiments that have been thought unfeasible at IBR-2 so far.

2. Scientific. In the 1999 scientific program for the IBR-2 spectrometers many of the performed investigations continued the themes that had become traditional for the Laboratoryг. In the past three years a program of investigations of a $HgBa_2CuO_{4+}d$ (Hg-1201) mercury-containing superconductor was carried out on the diffractometers HRFD and DN-12. It was precision investigations of the structure of the compound and how it changes under the action of high pressure at varying d or substitution of stoichiometric oxygen by fluorine atoms. In 1999 on HRFD a third member in a series of mercury-containing superconductors, $HgBa_2Ca_2Cu_3O_{8+d}$ (Hg-1223), was investigated in the condition when the main part of superstoichiometric oxygen was replaced by fluorine. The synthesis and certification of Hg-1223 were made in E. V. Antipov's laboratory of the Chemistry Chair of MSU. It is shown that a record temperature of the superconducting transition of 134 K obtained in oxygen-containing compounds increases to 138 K as fluorine is implanted. Another effect of fluorine doping is a noticeable decrease of the distance between copper and oxygen atoms in the conducting planes (CuO_2) without any increase in their corrugation. Finally, a neutronographic experiment made it possible to determine reliably the existence of atoms of stoichiometric fluorine in the center of the basis plane (HgO) and on the sides (*a*, *b*) of the cell. The latter may be related to partial substitution of mercury by copper atoms. (See Experimental Reports).

In 1998, a RRC Kurchatov Institute-MSU-FLNP collaboration conducted a series of experiments to determine the magnetic structure of a series of compounds, $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$, in which earlier there was observed a giant isotopic effect exhibiting itself as a change of the transport state (metal-dielectric) at low temperatures on substitution of oxygen isotopes (^{16}O by ^{18}O). In 1999, systematic structural data depending on the temperature and the mean radius of the A-cation were obtained for the series. An analysis of the data showed that mean values, such as the volume of a unit cell, the length of the bond <Mn-O>, and the valence angle <Mn-O-Mn> are linear functions of the Pr content or the mean radius of the A-cation, which is the same. The transition temperature to the metallic ferrmomagnetic state is also a linear function of the angle <Mn-O-Mn> (**Fig. 3**). One of the main goals of the work was to determine the structure of two samples with y=0.75 (LPCM-75) and different concentrations of ^{16}O and ^{18}O isotopes. A HRFD precision experiment made it possible to demonstrate that over the interval from room temperature to the transition temperature of samples with ^{16}O to the metallic ferromagnetic phase, $T_{FM, O\text{-}16}$, the investigated samples are identical not only in the parameters of the unit cell but also in the structure parameters, such as interatomic bond lengths and valence angles (**Fig. 4**). Reliable evidence of the fact that an essential difference in the transport and magnetic properties of the isotopically enriched samples LPCM-75 at $T < T_{FM, O\text{-}16}$ is due to different dynamics of oxygen atoms and as a result, unusually strong electron-phonon interaction was first obtained. (See Experimental Reports).

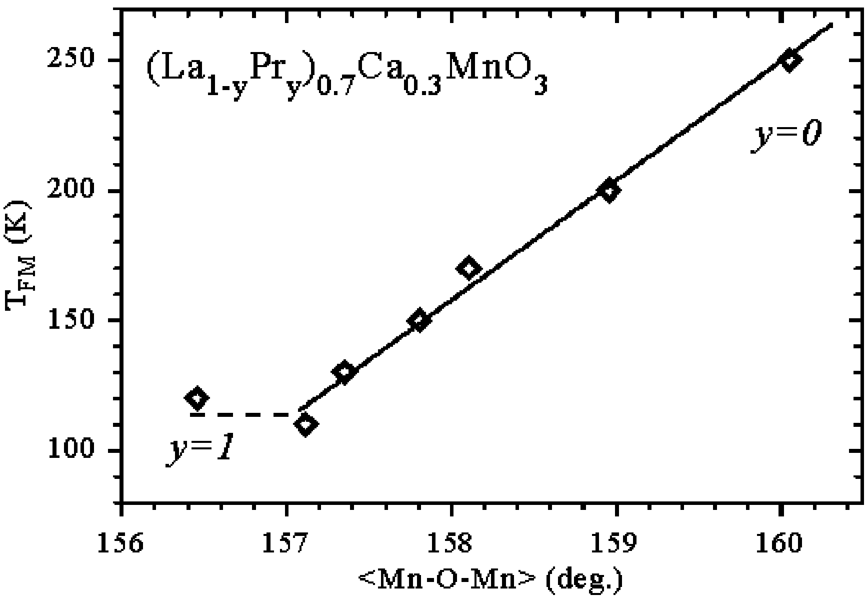
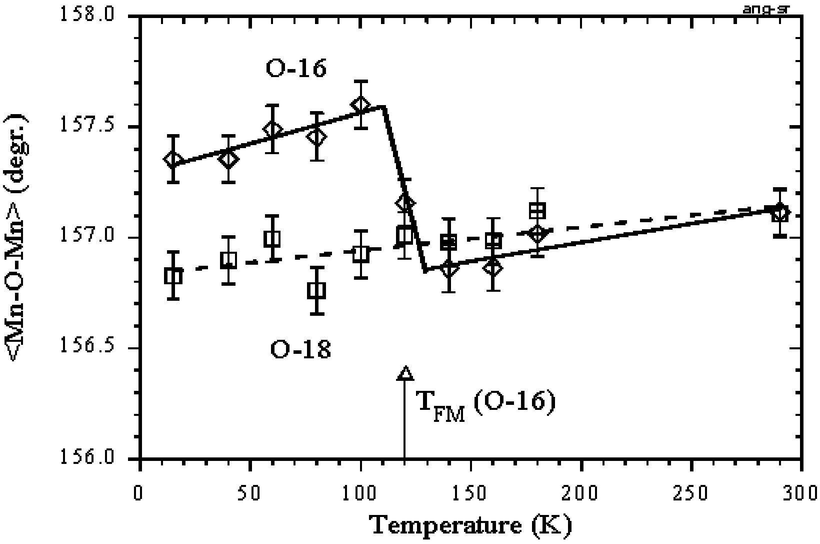


***Fig.** 3. The dependence of the temperature of the establishment of the far-range order FM on the mean value of the valence angle Mn-O-Mn.*

As soon as materials with a colossal magnetic resistance effect are interesting from the viewpoint of both fundamental and applied research, seeking new manganese oxide-based compounds is topical. In 1999 in E.V.Antipov's laboratory (Chemistry Chair, MSU) a $Ca_2GaMnO_{5+}d$ compound with a layered structure was first synthesized. In a neutronographic experi-ment conducted with the diffractometer DMC (SINQ) it was shown that compounds with the oxygen index 5.04 experience antiferromag-netic ordering below 150 K (**Fig. 5**) and the direction and value of the magnetic moments of Mn atoms were determined.

Helicoidal magnetic ordering in a Tb monocrystal was studied with the diffractometer DN-2. The aim was to investigate the influence of external axial of stretching on the spiral period and the intensity of satellite diffraction peaks. First, the temperature dependence of the magnetic structure was studied. **Figure 6** illustrates the temperature dependence of the vector of the spiral at normal pressure and it is seen that helicoidal ordering in Tb exists just in a narrow interval of temperatures, between 225 K and 231 K. Further measurements of the dependence of magnetic ordering on external axial stretching showed that the spiral disappears as the stretching gets larger than 400 bar. It is a strong argument for the assumption that the ordering depends on the form of the Fermi surface in metals which can be modified by external action.

On the diffractometer DN-12 there continued experiments to investigate the effect of high pressures on the structure of ammonium halides, particularly ND_4I, and search a possible structural transition at high pressure in SmB_6 In the latter case, experimentalists managed to observe anisotropic broadening of some diffraction peaks and even splitting of them which confirms the existence of the phase transition. To obtain more detail information, an experiment was conducted with the diffractometer POLARIS at the ISIS source. In the experiment to investigate the «electron» high temperature superconductor Nd_2CuO_4 structural changes and an accompanying interlayer transition of the charge at an external pressure up to 5Gpa were studied. A comparison of the contraction of separate interatomic distances in Nd_2CuO_4 with the contraction in «hole» superconductors revealed noticeable diffferences (See Experimental Reports).



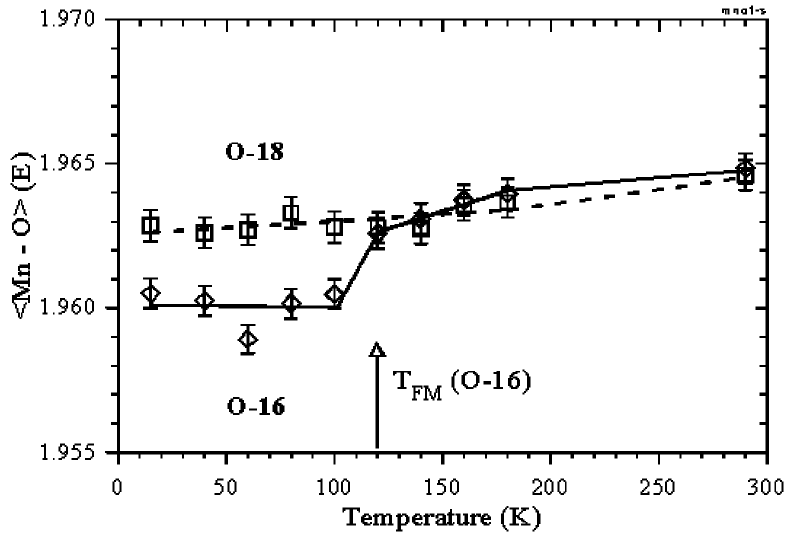


Fig.4. *A comparison of the temperature dependence of the mean length of the bond <Mn-O> (bottom) and of the mean valence angle <Mn-O-Mn> (top) for the samples* $(La_{0.25}Pr_{0.75})_{0.7}Ca_{0.3}MnO_3$ *with* ^{16}O *or* ^{18}O *isotopes. The arrow marks the transition temperature of the sample with* ^{16}O *to the FM-state.*

In 1999 the small angle diffractometer YuMO was intensely used to conduct investigations in different fields of biology, physics and physical chemistry. Also, experiments to study colloidal systems, polymers and solve problems in materials science were conducted. In particular, investigations of the behavior of surface-active substances under different conditions continued. In collaboration with Bayreuth University (Germany) the behavior of rod-like micelles in TMDMAO molecules was studied at different pressures and temperatures. Pressure-induced phase transitions at 280 K and 249.9 K were discovered. The difference between the chemical potentials of monomers in the edge and cylindrical parts of spherical-cylindrical micelles was determined. The difference between the chemical potentials of the monomers was determined.

Another example is a collaboration with the University of Utrecht (The Netherlands) for the investigation of a triple system, monoglyceride/dicedylphospate/water (MSG/DCP/water). It is of interest from the viewpoint of biology, the physics of accidental surfaces, and applied purposes (monoglycerides are basic alimentary emulsifiers). It is shown that even small amounts of charged lipid dicedylphosphate destroy an «infinite» bicontinuous minimal surface organized in an ordered cubic structure of the two-component system MSG/water. Topological and phase transitions were discovered in a wide temperature range of 10°C to 90°C for different mole ratios, MSG/DCP (19:1, 9:1,4:1), and lipid concentrations (DCP) in water (1, 10, 20, or 30 weight percent). An interesting effect was discovered:
polydispersion samples transformed into monodispersion ones. The influence of an air-sample interface on the properties of the given colloidal system was first proved.

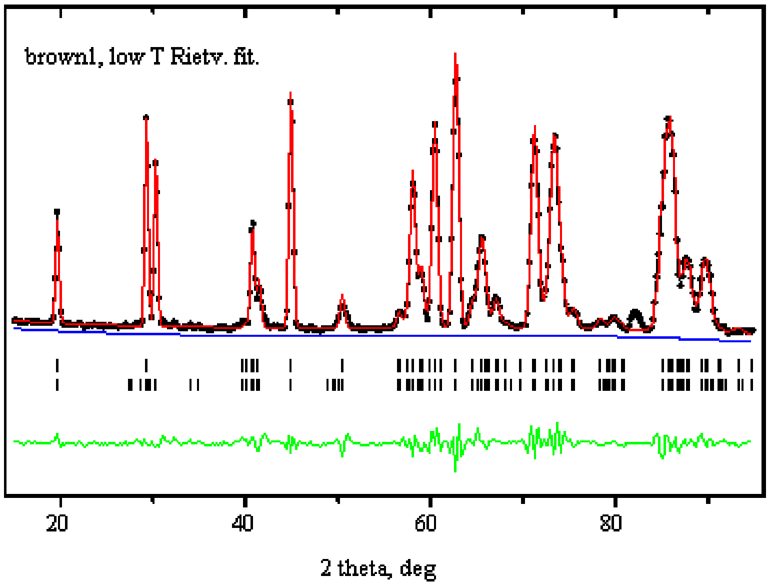


Fig. 5. *The diffraction spectrum of a $Ca_2GaMnO_{5.04}$ powder measured at T=12 K. Processing by the Rietveldt method is carried out taking into account the AFM-phase (the lower row of lines).*

An example of small angle neutron scattering investigations of biological systems is the study of purple membranes of (PM) of *Halobium Salinarium* bacteria. In experiments conducted together a research center in Juelich (Germany) there were discovered photo-induced changes in the structure of dopcyne (BR) protein, the only protein in PM. It is the very protein that catches a quantum of light and uses its energy to transport proton in an anti-electric potential gradient direction. The proton transport whose mechanism is not quite clear yet is a key element in the bioenergetics of cells. The conducted small angle scattering investigations showed that the polar part (loop) of BR is involved in proton transport-accompanying structural changes of the protein.

Systematic small angle neutron scattering studies of the properties of polymer systems started for the first time with YUMO. They were performed in collaboration with A. P. Khokhlov's laboratory of MSU. In particular, polymer gels with implanted surface-active substances were studied. For example, fractal arrangement of sodium dodecylsulphate (SDS) in a grid polymer from diallyldimethylammoniumchloride was discovered.

Investigations of layered structures continued on the spectrometer of polarized neutrons SPN using new experimental techniques - the observation of neutron standing waves and of neutron beam splitting at magnetization direction noncolinear with the interface of media. As a result, in the system Fe(1000 E)/Gd(50 E) there was observed triple spin-flip of the reflected neutrons (**Fig. 7**) and this was interpreted as neutron spin-flip at transmission through two domain walls enveloping the magnetic domain. To verify the hypothesis, model calculations will be carried out.

The most interesting result obtained with the reflectometer of polarized neutrons REFLEX was a new estimate of the upper limit of the neutron coherent wavelength manifesting itself in the process of neutron specular reflection from thin films. The experiment consisted of precision measurements of the reflection curve R(l) from a thin film of Cu (~1800 E) on a glass substrate and its description with an analytical function. It appears that the quality of the reflection curve description improves essentially as one introduces in the formula for R - parameter which in particular, can be interpreted as a quantity related to the coherent properties of the neutron wave. In this interpretation the estimate of the neutron coherent wavelength is 1.5 mm which is approximately 8 times larger than published earlier in the literature. In any case, the experiments showed that the description of precision reflectometric data should be modified and this may be important for their interpretation in a number of cases.

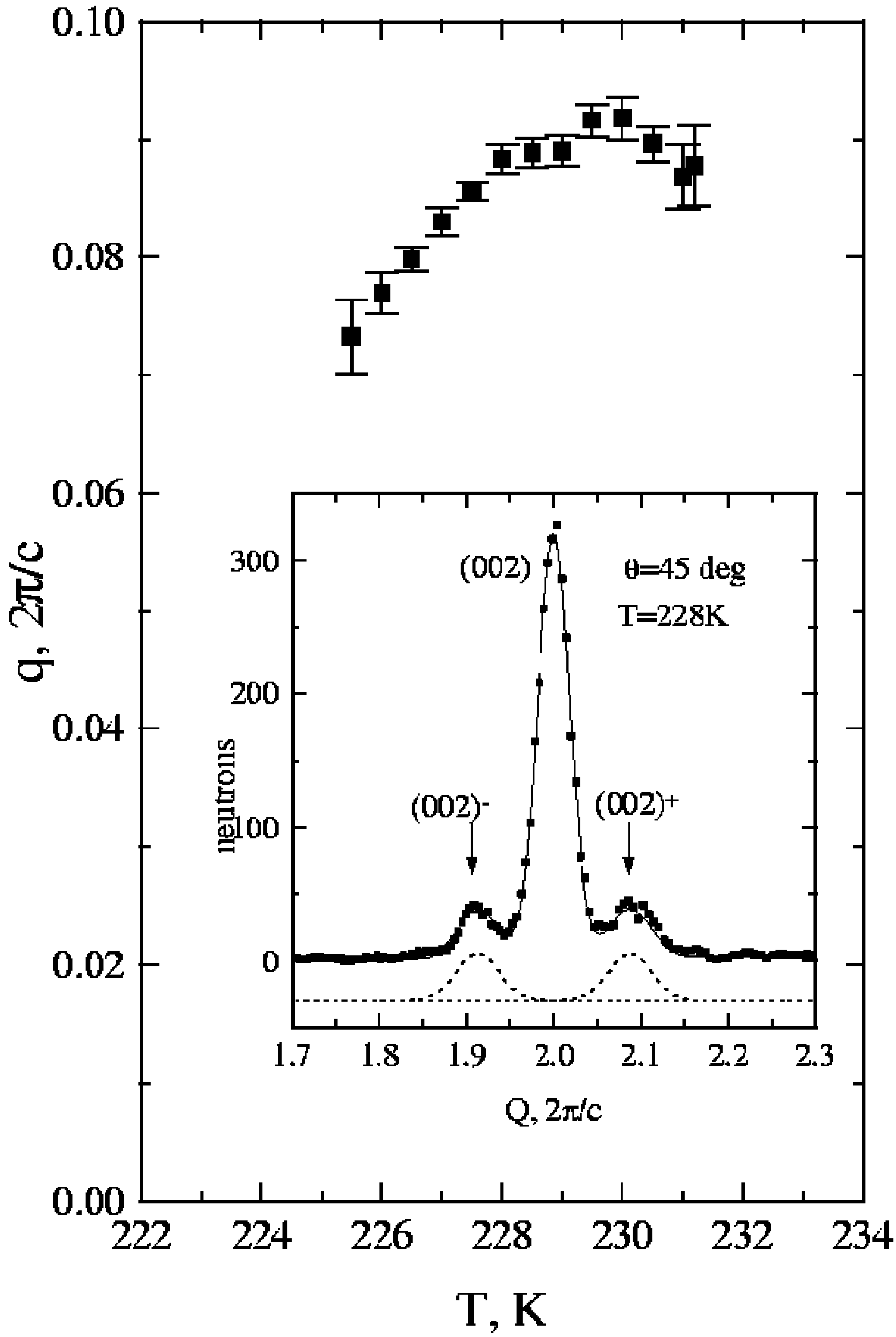


Fig.6. *Temperature dependence of helicoid magnetic structure in Tb. Helicoid arrangement exists only in narrow temperature diapason from 225 to 231 K. A typical part of diffraction spectra are shown in the inset.*

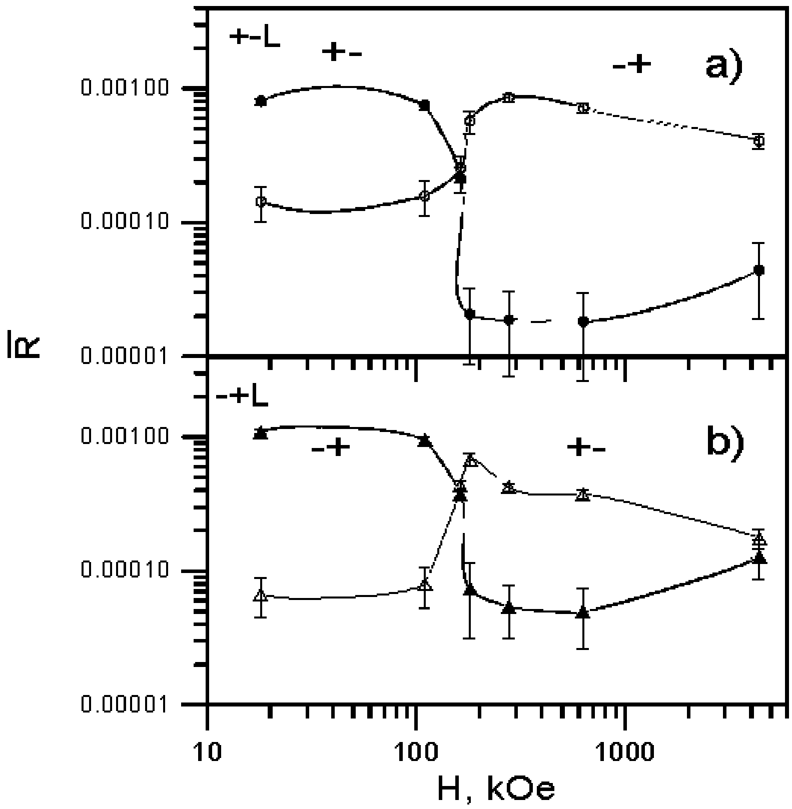


Fig. 7. The dependence of the neutron reflection coefficient R on the external magnetic field H for «+-« and «-+» spin transitions, «+-L» and «-+L» spin transitions in a local surface magnetic field.

The main direction of research on the inverse-geometry spectrometer NERA-PR was the investigation of the dynamics of ammonium groups and their influence on structural phase transitions in ammonium salts. In particular, in 1999 there continued experiments to study $Rb_{1-x}(NH_4)_xI$, $K_{2-x}(NH_4)_xSeO_4$, $LiRb_{1-x}(NH_4)_xSO_4$, and $Rb_{1-x}(NH_4)_xMnF_3$. Transitions to a proton (orientational) glass phase at low temperatures and a transition to the ordering of ammonium groups with increasing concentration of ammonium were investigated. The crystalline-to-glass phase transition in solid methanol phases CH_3OH, CH_3OD, and CD_3OH, i.e., for different numbers of deuterium atoms in the molecule, were also investigated.

An extended program of experiments was carried out with the DIN-2PI spectrometer. In particular, investigations of water solutions to reveal the effect of dissolved particles on the microdynamics of water molecules entering into the hydrate spheres of the particles continued. Detail knowledge of the phenomenon which has been given the name of hydration is essential in the physics of solutions lying in the basis of the most important directions of chemistry, biology, and related sciences. Constantly growing interest in hydrophobic effects is practical and comes from the role they play in the organization and functioning of the most important biological structures (cell membranes, proteins, etc.) and of surface-active substances (micelles, emulsions). An analysis of DIN-2PI experiments shows that in contrast to small ions (Li^+ and Cs^+) large apolar particles do not destroy the grid of hydrogen bonds in their surrounding water. The next step to the understanding of the discussed phenomena is to search a relationship between the obtained microscopic information and the known macroscopic thermodynamic hydrophobic effects.

Also, low-frequency vibrational modes of atoms in the normal and superionic phases of PbF_2 at T=293 or 823K were investigated with DIN-2PI. The obtained data provide evidence in favor of a liquid-like state of the anion sublattice in the superionic phase of PbF_2 the nature of collective excitations of which is different from classical liquids. At the same time, investigations of hydrates, including the system $Zr\text{-}H_x$ (x=0.38-0.80) in particular, continued. In samples with a low hydrogen content in the energy transfer interval 2-10 meV the system exhibits low-frequency excitations possibly connected with tunneling or resonance effects in the dynamics of hydrogen atoms in a-Zr.

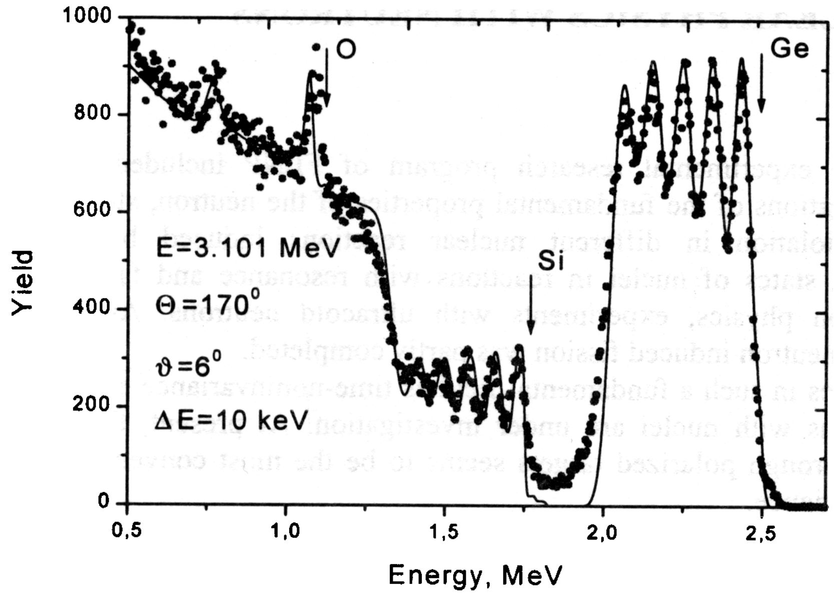


Fig. 8. The experimental (points) and calculated (line) RBS spectra for a 10-layer Si/Ge structure. The layer thickness: Si-23nm, Ge-13nm. The presence of oxygen in the layers is also detected (13 atomic %).

The conducted applied research was mainly the investigation of internal stresses in large-volume products with the spectrometers HRFD and EPSILON, of rock textures with the spectrometer SKAT, and the application of diagnostic methods at an ion accelerator (see Experimental Reports). The important feature of the 1999 year is the beginning of real cooperation with several industrial plants in Russia which approached the Laboratory on the matter of conducting internal stress investigations of key parts in different machines. Investigations of Ge/Si layered structures aimed, in the main, at the determination of the amount and positions of oxygen in the layers continued at the accelerator EG-5 under the auspices of the program «Ion Beams for the Certification of Semiconducting Materials» with the support of IAEA (fig.8).

Scientific program of the Condensed Matter Physics Division in 1999 was executed in cooperation with the following institutes and organizations

Bulgaria	University; Institute for Nuclear Research and Nuclear Energy (Sofia)
Czech Republic	Polytechnical Institute (Prague)
Egypt	Atomic Energy Authority of Egypt (Cairo)
Finland	Technical Center (Espoo)
France	Laboratoire Leon Brillouin (Saclay); Institut Laue-Langevin (Grenoble)
Georgia	University (Tbilisi)
Germany	Hahn-Meitner Institute (Berlin); Research Center (Rossendorf); University (Bayreuth); Technical University (Kemnitz); Research Center (Darmstadt); GKSS (Geesthacht); Fraunhofer Institute for Nondestructive Testing (Dresden-Saarbruecken)
Hungary	Research Institute for Solid State Physics (Budapest)
D.P. Republic of Korea	University (Pyongyang)
Poland	Institute of Nuclear Physics (Cracow); University (Poznan)
Romania	Atomic Physics Institute (Bucharest)
Russia	Kurchatov Institute; Institute of Solid State Physics; Institute of Theoretical and Experimental Physics; Petersburg Nuclear Physics Institute; Institute of Physics of Metals; Moscow State University; Institute of Crystallography; Physical Energetical Institute (Obninsk); Institute of Nuclear Physics RAS
Slovakia	University (Bratislava)
Sweden	University (Goteborg)
Switzerland	Paul Scherrer Institute (Villigen); ETH Zentrum (Zurich)
U.K.	Rutherford Appleton Laboratory (Abingdon)
Uzbekistan	Institute of Nuclear Physics (Tashkent)
Vietnam	Institute of Physics (Hanoi)