1.1. CONDENSED MATTER PHYSICS

In accordance with theme -0864- neutron scattering investigations in the field of condensed matter physics are conducted at IBR-2 using four main experimental techniques: diffraction, small-angle scattering, inelastic scattering, and polarized neutron optics. Beam time is allocated according to experts recommendations based on submitted proposals and the existing long-term agreements for co-operation.

Spectrometers for investigations in condensed matter physics. To the experimental halls of the IBR-2 reactor 14 neutron beams are extracted and physical instruments are arranged on them. At present, 12 spectrometers are for condensed matter investigations. In 1997, nine of them were operating in the user mode: HRFD, DN-2, NSVR, YuMO, SPN, REFLEX-P, KDSOG, NERA, and DIN. The DN-12 spectrometer had undergone radical modernization completed by the summer of 1997. Following PAC recommendations the SNIM spectrometer was excluded from the user program for 1997. The DIFRAN spectrometer operated in the frame of a special program.

For the most part, the main parameters of spectrometers included in the IBR-2 working schedule have been formed and on the whole, they are on the world level. At the same time, work to expand the possibilities of several instruments was conducted in 1997.

The parameters of the DN-12 diffractometer for experiments with high pressure cells based on sapphire or diamond anvils were essentially improved by introducing a new neutron guide. This curved 20 m supermirror neutron guide gave a double increase in the total thermal neutron flux and at the same time, a several times increase in the flux of neutrons with $\lambda>2$ E (Fig. 1) and a sharp decrease in the background (see Sec. Experimental Reports).

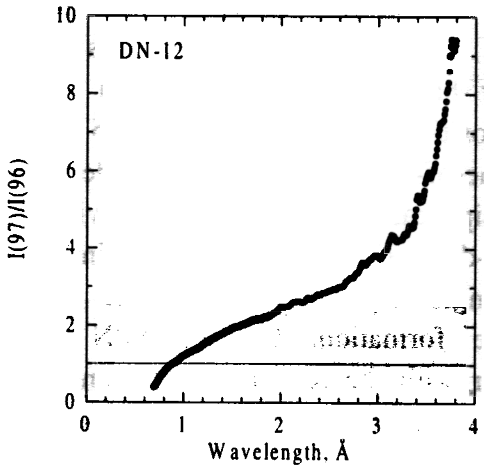

Fig.1. An increase of the neutron flux on the sample after installation of the supermirror neutron guide in the DN-12 diffractometer.

Another event of equal importance was putting into operation of the SKAT spectrometer in place of the NSVR spectrometer that had operated over 10 years at IBR-2. The detector system for SKAT arranged in the vertical plane made it possible to optimize essentially the registration of pole figures in investigations of bulk sample textures, have shorter measuring times as well as improve the quality of measurements.

On the high resolution Fourier diffractometer (HRFD) a second detector at $2\theta=-152°$ was put into operation. This reduced the time of structure experiments two times. Final adjustment of the detector elements decreased the geometrical component of the resolution function. This reduced the relative width of the resolution function to 0.12% for $d=1.5$ E and the rotation velocity of the chopper 8000 rpm. In Figure 2 diffraction spectra measured with HRFD and the TOF-diffractometer HRPD at ISIS with the flight path 100 m are compared. One can see that in spite of the fact that HRFD has an approximately 5 times shorter flight path the resolutions of these spectrometers are about equal.

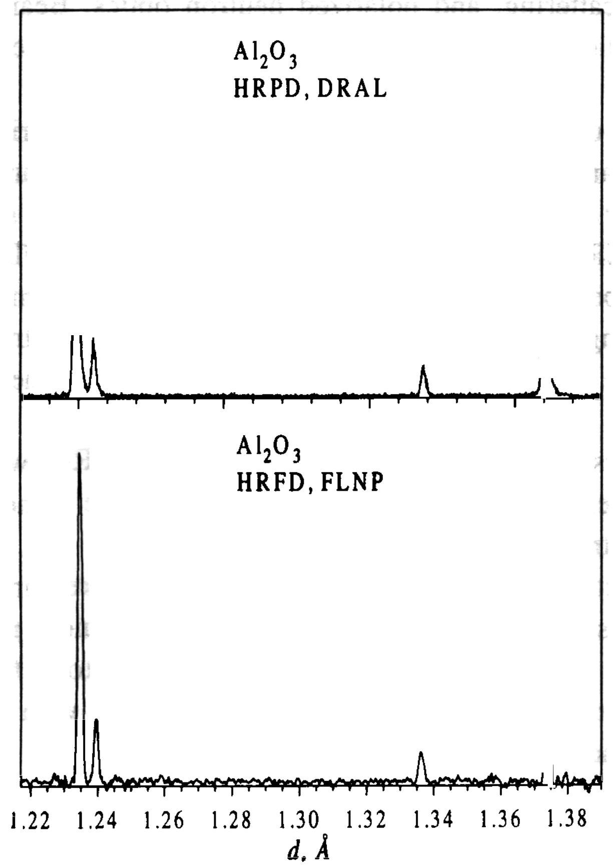

Fig.2. The part of the diffraction spectrum from one Al_2O_3 sample measured with HRPD (ISIS) and HRFD (IBR-2) diffractometers .

In 1997, work to improve position-sensitive detectors was carried out. The possibilities of the DN-2 diffractometer have noticeably increased after a two-dimensional detector (320x280 mm^2) with the position resolution about 2.5 mm in two coordinates started operation. In addition to time-of-flight analysis, this detector allows registering the three-dimensional scattering in the reciprocal space of the crystal without rotating the sample or the detector. Figure 3 illustrates a tow-dimensional distribution of intensity in one of the reciprocal lattice sites in a La_2CuO_4 single crystal following the tetragonal to orthorhombic phase transition and twin structure formation. On the SPN spectrometer experiments using a linear position-sensitive detector with the resolution 1.5 mm started. This detector registers the reflected neutron distributions in the SPN reflectometric mode and can be also used to realize the SPN small-angle mode.

Execution of the scientific program. From 1995 the scientific program for investigations with the IBR-2 spectrometers is formed, in the main, on the basis of proposals submitted to experts commissions by users from JINR member states (10% from other countries). About one half of proposals is for investigations under auspices of long-term agreements for cooperation between FLNP and other laboratories or institutes in investigation of particular problems of condensed matter physics.

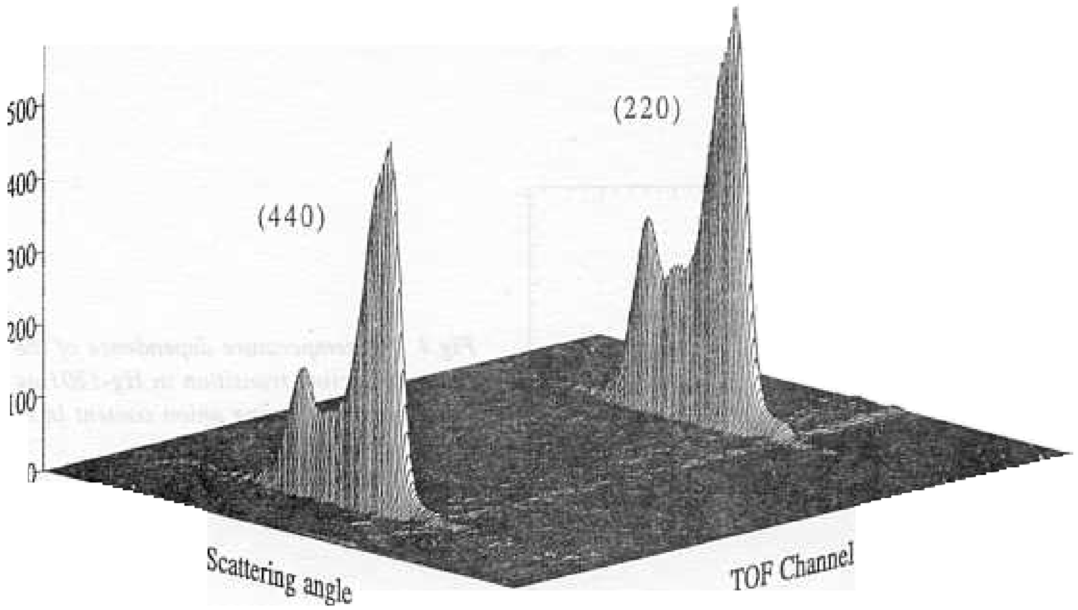

Fig.3. Neutron diffraction pattern along of (hh0) direction of a La_2CuO_4 crystal (in the ferroelastic phase), measured with a two-dimensional PSD and summed over vertical coordinate of the detector.

Diffraction experiments. The program for investigations of mercury based high temperature superconductors carried out in collaboration with the Department of Chemistry of Moscow State University (MSU) continued and extended to studies of the atomic structure of the compound $HgBa_2CuO_4F_\delta$ i.e., the compound with extra oxygen replaced by fluorine atoms. The idea of the experiment is to replace a bivalent doping element by a monovalent element. In this case, the conservation of the charge balance and the ionic nature of carriers formation require doubling the amount of doping atoms to have an equivalent superconducting transition temperature. The *Hg-1201* initial phase with T_c=61 was successfully fluorinated with XeF_2 in MSU (E.V.Antipov's laboratory). As a result, T_c increased initially to 97 K and then decreased which was followed by suppression of superconducting properties as the fluorine content in the sample increased. A neutron diffraction analysis of two $HgBa_2CuO_4F_\delta$ compositions (experiments with HRFD at IBR-2 in May 1997) confirmed the implantation of fluorine in the charge reservoir (*Hg*-plane) and really showed the doubling of the fluorine content in the structure in comparison to *HG-1201* oxygen phases with close T_c (Fig. 4). This is a strong argument in favor of the ionic model of electric charge carriers (holes) formation in *Hg*-1201 in the process of doping (see Sec. Experimental Reports).

To investigate the phenomenon of macroscopic phase separation in superconducting crystals, a series of experiments to study the transformation twinning in $La_2CuO_{4+\delta}$ crystals were conducted with the DN-2 diffractometer. Concurrently, experiments with the *X*-ray diffractometer of ISSP (Chernogolovka) were carried out. In the DN-2 experiments the new position-sensitive detector was used. The measurements demonstrated that the domain (twin) structure in such crystals is noticeably different from the classical scheme realized at a loss of an axis of the 4th order and observed in KDP crystals or *Y-123*. It appears that the boundaries between domains are mainly coherent (the portion of domains with incoherent boundaries is not large). Moreover, in crystals where macroscopic phase separation takes place this portion is not larger than a few percent. This, possibly, leads to extra oxygen diffusion and, as a result, to separation.

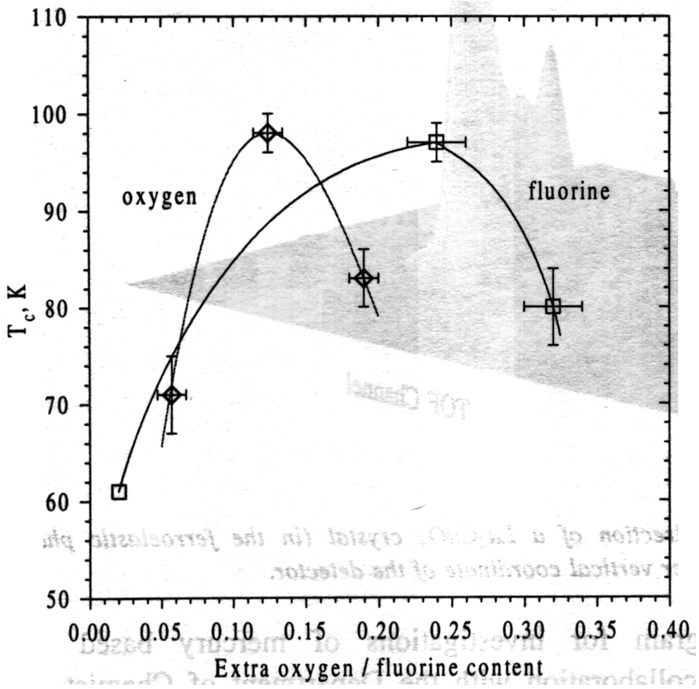

Fig.4. The temperature dependence of the superconducting transition in Hg-1201 as a function of the doping anion content in the cases of oxygen or fluorine doping.

Studies of the magnetic state of crystals in both neutron and μSR experiments yield interesting results. During 1997, a number of such investigations were performed using the μSR spectrometers in the Meson Factory in PSI (Villigen, Switzerland). One of the compositions of the system $U(Pd_{1-x}Fe_x)_2Ge_2$ studied earlier in detail by means of neutron diffraction was investigated on the GPD spectrometer over a wide temperature interval. It is discovered that muon spin precession takes place at not only one but two and even more frequencies (Fig. 5). An analysis proves that this is connected with the existence in an elementary cell of the compound of equivalent crystallographic positions which are nonequivalent from the point of view of the magnetic surrounding (see Sec. Experimental Reports).

Another example of analysis of combined neutron and μSR data is the results obtained for $La_2CuO_{4+\delta}$ single crystals with the doping level δ=0.02-0.03, i.e., lying inside the miscibility gap but having a reduced coefficient of oxygen diffusion. According to neutron data the long-range order with the coherent length large enough to observe the magnetic diffraction peaks is established either in a small volume portion (~10%) of the crystal or is not established at all. At the same time, μSR data are evidence of the fact that in the superconducting phase transition point or its vicinity there arises the magnetic order sufficient to observe muon spin precession. These results can be interpreted as the appearance of separation into the superconducting and antiferromagnetic phases that occurs on the electron level in regions small in size and is induced by the superconducting state transition (see Sec. Experimental Reports).

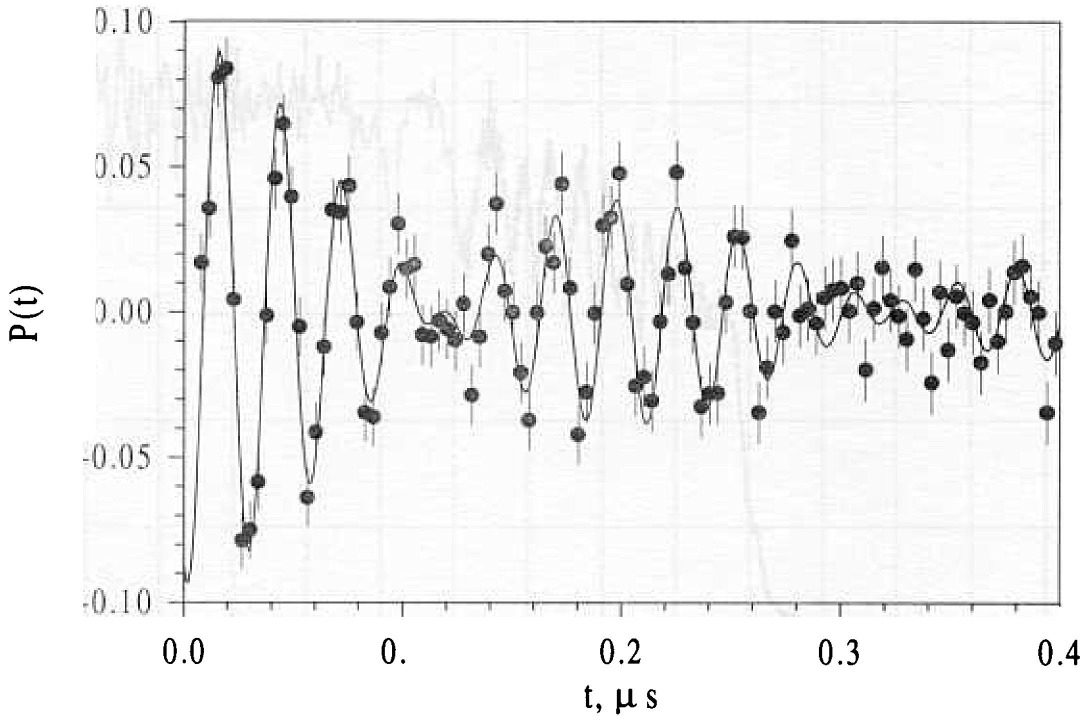

Fig.5. *The time dependence of the muon spin polarization function in the* $U(Pd_{0.99}Fe_{0.01})_2Ge_2$ *at 13K measured by μSR-spectroscopy. The polarization reflects the muon spin precession around internal magnetic fields in the sample. The presence of characteristic beats is due to the existence of two or more precession frequencies.*

FLNP in collaboration with IBC (Moscow), ISSP (Budapest) and LURE (Orsay) investigated the vesicle transition in the system phospholipin/sodium cholate/water with the YuMO spectrometer. Morphological and structural changes following changes in the temperature or the detergent concentration were studied. In a dimyristylphospatydilcholine-based system the transition from the multilamellar structure to the unilamellar structure formed through the stage of elongated rod-like micelles formation was observed. Also, an analysis of SANS data allowed determination of the geometrical characteristics of the formed micelles.

The first experiments of generating and registration of neutron standing waves were carried out on the SPN spectrometer. Developing the method may prompt the solution of the problem of the determination of the structural positions of atoms in the near-surface region of matter. In the experiment the dependence of the intensity of γ-quanta emitted following neutron capture in a thin gadolinium layer (~50 E) deposited on a magnetized Fe layer (~1000 E) on the incident neutron beam polarization was registered. The preliminary analysis of the measured dependence allows us to speak about an observation of a standing neutron wave with about 90% probability (see Sec. Experimental Reports).

Concurrent with detailed certification, on the new polarized neutron reflectometer REFLEX experiments to study the properties of some neutron-optical systems, such as multilayer mirrors produced by PINP (Gatchina) and CIFI (Budapest), the interference filter for the UCN spectrometer (Dubna-Grenoble-Melbourne collaboration), etc. were carried out. A high resolution of the reflectometer which is probably the record one today makes it possible to obtain information about fine details of surface layers (Fig. 6).

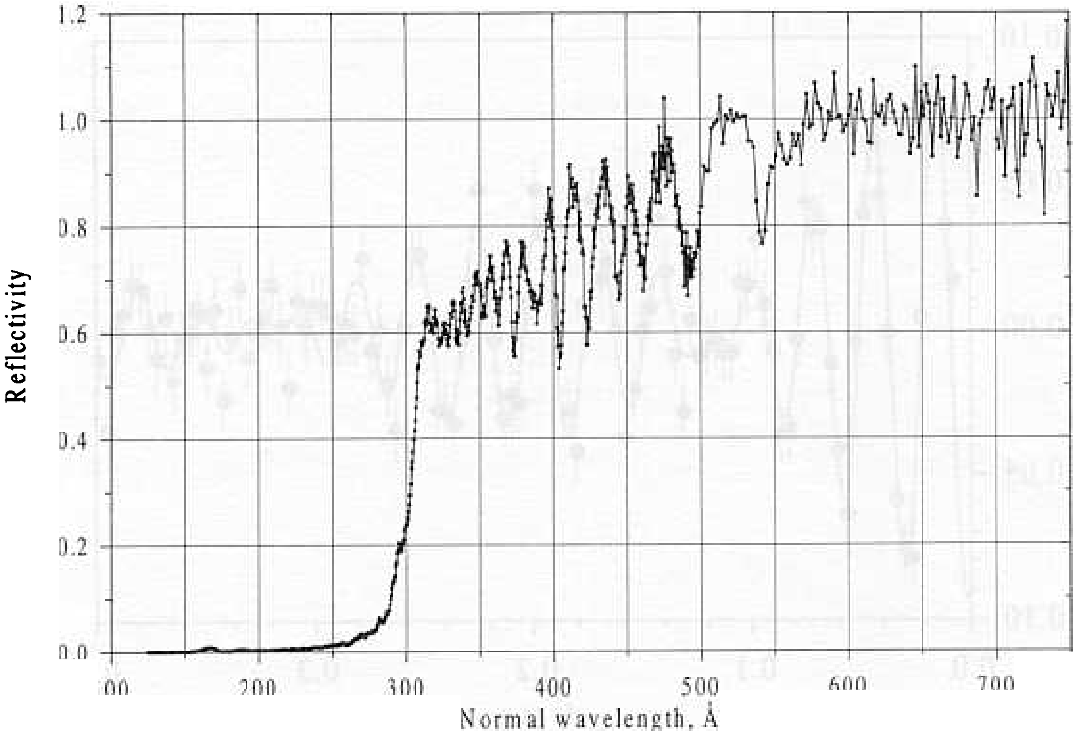

Fig.6. *The reflection coefficient of neutrons from multilayer mirrors. The modulation of the reflection coefficient is due to fine details of the surface layer.*

The main research direction on the NERA spectrometer was the study of the dynamics of ammonium and methyl groups at phase transitions in stoichiometric compounds of the type $(NH_4)_2SO_4$ and solid solutions of the type $(NH_4)_{2-x}Rb_xSO_4$. Replacing ammonium ions by Rb with about equal ionic radius leads to some disorder in the system of hydrogen bonds and allows investigation of the influence of disorder on the dynamics of ammonium. The system $(NH_4)_{2-x}Rb_xSO_4$ was investigated over the entire concentration interval $(0 \le x \le 2)$ for a wide temperature range $(10 \le T \le 300\ K)$ by neutron diffraction, inelastic and quasielastic scattering. This has made it possible to complete the determination of the phase diagram of the compound on which the critical transition point to the ferroelectric phase was found. The registered inelastic scattering spectra were used to verify the macroscopic model of the dynamics of such crystals. The model yields a satisfactory explanation for the mechanism of the observed phase transitions and the role of ammonium dynamics in the formation of the ferroelectric properties of crystals (see Sec. Experimental Reports).

In 1997, on the KDSOG spectrometer largely increased the number of external users and consequently, the number of solved problems, including, in particular, the measurement of crystalline fields in HTSC and CMR materials, determination of phonon spectra in ferroelectrics, Ni_3Al-based intermetallic compounds, isotope substituted amorphous alloys in the system Zr-Ni and nitrous steels, and the study of hydrogen vibrations in nonequilibrium ω-Ti and Zr, the intermetallic compound $FeTi$, and complex carbo- and nitrohydrates. One of the interesting results obtained is the discovery of a change in the magnetic response following the doping of the compound $AlSr_2Er_{1-x}Ca_xCu_2O_7$ *(1212)*. This allowed constructing the model of charge redistribution in the CuO_2 planes. There are plans for carrying out experiments to verify the model over a wide doping range.

On the DIN spectrometer investigations in traditional directions, such as the atomic dynamics of liquid metal systems with gas admixtures, relaxation characteristics of liquid helium, hydrogen dynamics in triple implantation systems based on transitional metals of the V-group, continued and were aimed at refining and systematization of the earlier obtained data.

Applied research was actively conducted on the HRFD diffractometer (investigations of internal stresses in bulk samples, determination of the structure of activated catalysts) and the NSVR diffractometer (textures of geological materials).

In particular, Al_2O_3/Al composites with a ceramic matrix were studied with HRFD. The development of the technology of production of new materials has led to the new method of manufacturing composite materials by infiltrating metals into a porous ceramic matrix by means of gas pressure and formation of a deep grid microstructure. In this case, fragile ceramic materials are strengthened by introducing the elastic phase using metals, as a rule. This makes it possible to improve the mechanic characteristics of composites. Usually, a metal is infiltrated into the matrix at temperatures a little higher than the melting temperature of the metal. The typical materials of that kind are Al_2O_3/Al composites where the metallic Al phase is infiltrated in the porous ceramic α-Al_2O_3 matrix. Residual stresses in Al_2O_3/Al composites arise as a consequence of an essential difference between the coefficients of thermal expansion of two phases (for Al_2O_3 - $\alpha=8.3\times10^{-6}$ °C^{-1}, for Al - $\alpha=22.5\times10^{-6}$ °C^{-1}). On HRFD two series of Al_2O_3/Al composites with the average size of metallic implants 0.1 μm or 1 μm were investigated. In each series the porosity of the matrix and correspondingly, the volume portion of Al is 15%, 25%, or 35%. An intensity analysis of Al reflexes demonstrates the existence of a strong texture in the metallic phase and the absence of a preferred orientation in the Al_2O_3 phase (see Sec. Experimental Reports).

Scientific program of the Condensed Matter Physics Division in 1997 was performed 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)
Slovakia	University (Bratislava)
Sweden	University (Goteborg)
Switzerland	Paul Scherrer Institute (Villigen)
U.K.	Rutherford Appleton Laboratory (Abingdon)
Uzbekistan	Institute of Nuclear Physics (Tashkent)
Vietnam	Institute of Physics (Hanoi)