1.1. CONDENSED MATTER PHYSICS

Scientific results. Diffraction. The work started in 1997 to investigate doped manganese oxides of the type $La_{1-x}Ca_xMnO_3$, $0 \le x \le 1$, where a certain level of doping triggers the Colossal MagnetoResistance Effect, continued. The effect consists of a dramatic decrease of the electric resistance of the material if an external magnetic field is applied. The reason of the decrease is the phase transition from dielectric to metallic state. The CMR effect may reach a value of 10^7 and higher. Applications of such compounds in technology will be diverse and their effectiveness may be extremely high. In the year 2000, the main direction of research in CMR-materials was carrying out of experiments to obtain information on how homogeneous the states arising at transition from dielectric to metallic phase are. Starting from the classical paper of Wollan and Koehler (Wollan E., Koehler W. *Phys. Rev.* **100** (1955) 545) simultaneous presence in the diffraction patterns of some perovskite manganites of both AFM and FM intensities is interpreted either as a uniform non-collinear (canted) magnetic phase or a spatially separated two phase state: AFM-dielectric and FM-metallic. To choose an acceptable variant for $LaMnO_{3-\delta}$ they carried out experiments in the magnetic field. On the basis of the fact that the dependence of the magnetic AFM and FM intensities on the field strength is non-correlated they came to the conclusion that the low-temperature state is a two-phase state. In the year 2000, similar experiments to investigate one of the canonical CMR compounds $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ (LPCM-*y*) were conducted (in collaboration with N.A.Babushkina (RRC KI), A.R.Kaul MSU) and P.Fischer (PSI)) for $y=0.75$ and 0.9 being on different sides of the boundary between the metallic and dielectric state. The experiments were done on the diffractometer DMC in an external magnetic field of up to 4 T at the temperature 4 K in PSI (Switzerland). It appears that the behavior of LPCM-75 in the field is analogous to that of $LaMnO_{3-\delta}$ (**Fig.1a**) but the intensity of LPCM-90 peaks changes in a strictly synchronous manner (**Fig.1b**). The experiments contributed essential additions to the phase diagram of LPCM-*y* and helped determine its basic states. Namely, at $y<0.60$ corresponding to the average radius of the A-cation $r_A>1.190$ Å, the LPCM basic state is a homogeneous metallic state with a ferromagnetic ordering. If $y>0.85$, i.e. $r_A<1.182$ Å, the basic state of LPCM is also homogeneous in the main but the type of conductivity is semiconducting and the magnetic moments of manganese form a noncollinear antiferromagnetic structure. In the intermediate region of r_A values there arises a mixed state with spatially separated domains of the mesoscopic size (~1000 Å) demonstrating different types of conductivity and magnetic structure. The physical reasons of formation of a two-phase state in magnetic manganese oxides are the object of further experimental and theoretical research.

In the year 2000, besides LPCM there were investigated other manganese compounds. In particular, preliminary experiments to determine the atomic and magnetic structures of $(Nd,Tb)_{0.55}Sr_{0.45}MnO_3$ and $(Nd,Sr)(Mn,Ru)O_3$ (together with A.Kaul's laboratory, MSU), Ca_2GaMnO_5 and Sr_2GaMnO_5, (together with E.Antipov's laboratory, MSU), study dimensional effects in nanocrystalline samples of $LaMnO_{3-\delta}$ (together with IFM, Ekateringurg), etc. were made.

In particular, the magnetic structure of the $(Nd,Tb)_{0.55}Sr_{0.45}MnO_3$ compound at the lowest temperature reached (~11.4 K) is quite complicated. It includes the ferromagnetic order in the sublattice of Mn cations and the ferrimagnetic order in the lattice of rare-earth cations (Nd,Tb). The magnetic moments of Mn ions are aligned along the *c*-axis of the Pnma unit cell. For the ferrimagnetic sublattice of rare-earth ions, its ferro-component is aligned strictly in the same direction as the Mn-ions moments are aligned, while the antiferro-component is aligned along the *a*-axis, formally forming a «G-type» antiferromagnetic ordering structure (all rare-earth neighbours of the given RE ion do have spins in the opposite direction). The transition temperatures of these two sublattices are not equal (**Fig.2**).

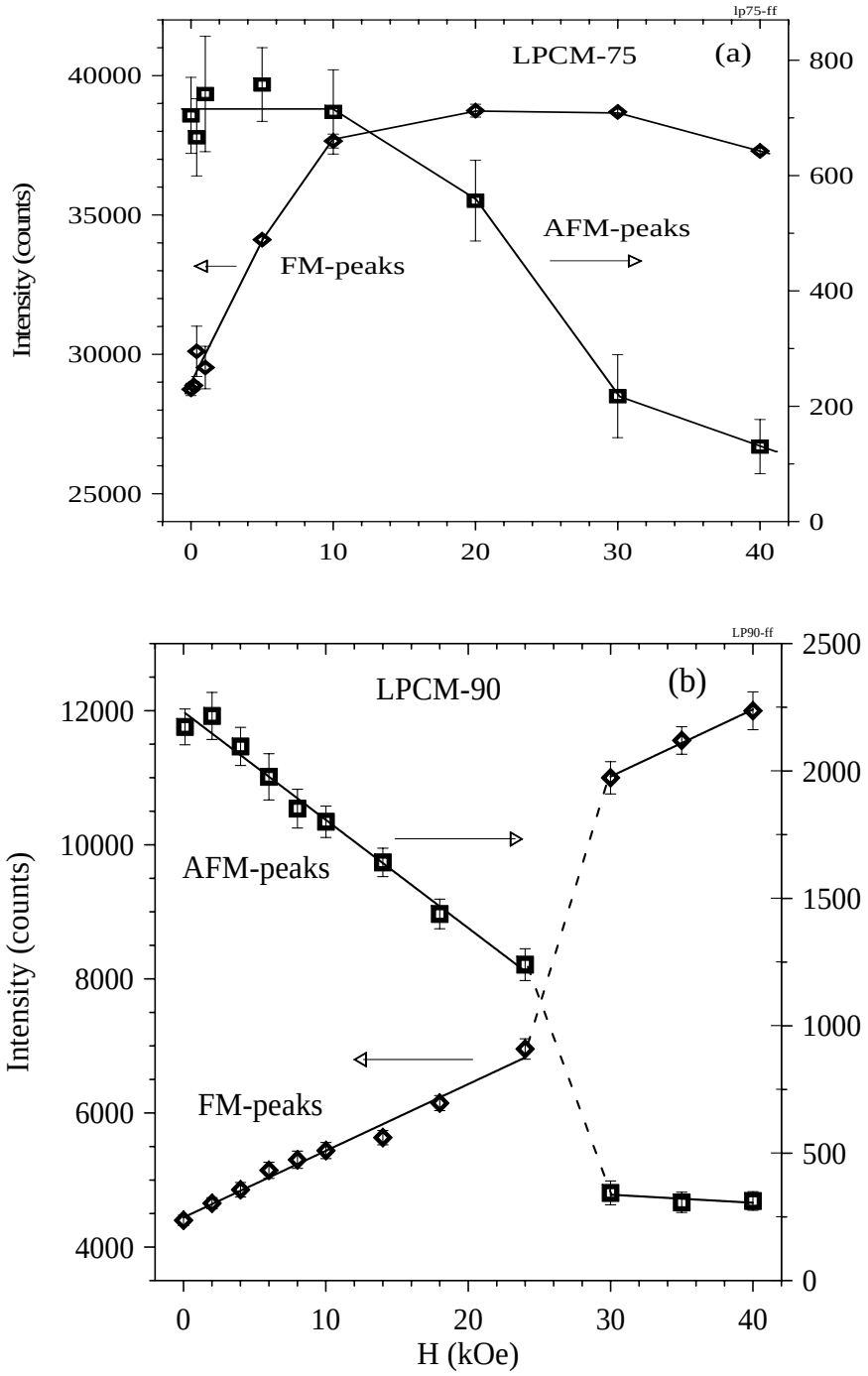

Fig.1. *The dependence of the FM- and AFM-peak intensity on the magnetic field for compositions with y=0.75 (a) and 0.90 (b). In the compositions with y=0.75 changes in the intensity do not demonstrate a synchronous behavior while in the compositions with y=0.90, they are synchronous. In the first case, the sample is in the two-phase state and changes in the intensity of AFM peaks only start to occur at sufficiently large fields. In the second case, the FM- and AFM components are related through the slope angle whose changes lead to synchronous changes of the intensity of peaks.*

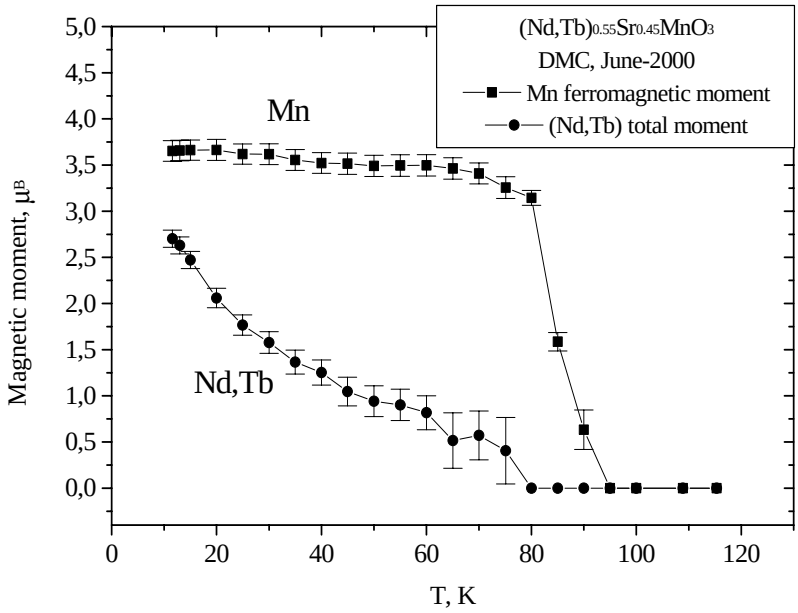

Fig. 2. *The temperature dependence of Mn and rare-earth cations (Nd,Tb) in the compound* $(Nd,Tb)_{0.55}Sr_{0.45}MnO_3$ *as measured in the neutron powder diffraction experiment.*

In the last few years in FLNP investigations of phase separation and magnetic ordering in $La_2CuO_{4+\delta}$ single crystals are conducted. Combined neutron diffraction and μSR experiments (V.Yu.Pomjakushin et al., Phys. Rev. B 58 (1998) 12350) showed that superconductivity and long range magnetic order coexist in these crystals and in addition, in $La_2CuO_{4+\delta}$ crystals with a low oxygen mobility the transition temperature to the superconducting phase coincides surprisingly with that to the static AFM phase. The problem is presently being solved in the framework of the hypothesis of the so-called microscopically phase separated state. It is however not clear yet whether the arising of a spatially inhomogeneous state favors the appearance of superconductivity or on the contrary, the two processes compete. In the year 2000, there were undertaken careful investigations in search of long range magnetic ordering, i.e. the one observed in the diffraction experiment, in a $La_2CuO_{4.02}$ single crystal with T_c=15 K where, as it is found by A.M.Balagurov et al. (Physica C, 272 (1996) 277), no macroscopic separation into phases with a high and low oxygen content exists. It has been shown that down to 2 K, the long range AFM order is absent in this crystal although from the μSR data it follows that the static magnetic order sets on at the temperature equal to T_c. The plans of further investigations into the problem include fluorination experiments of $La_2CuO_4F_\delta$ whose fluorine content may exceed the amount of additional oxygen several times.

On the diffractometer DN-12, investigations of the structure of triple compounds of mercury chalchogenides $HgSe_{1-x}S_x$ at x=0.3, 0.5, 0.6 and an external pressure of up to 3 GPa were conducted (in collaboration with IFM, Ekaterinburg). The extreme terms in the series HgS (x=1) and HgSe (x=0) have essentially different crystalline structures and crystallize in hexagonal and cubic syngonies, respectively. Of interest is to know the influence of pressure on the structure of mixed compounds. In the compound with x=0.3 the phase transition from cubic zinc-blend phase to hexagonal cinnabar phase occurs at P≈1 GPa, the jump in volume being about 12%. The dependence of the hexagonal phase parameters on the pressure is obtained.

On the diffractometer DN-2, structural modulation peculiarities in a single crystal of the ferroelectric-semiconductor $TlInS_2$ were studied in collaboration with several groups from Japan (see Experimental Reports). In the experiment, three-dimensional distributions of the scattered neutrons along the directions [100] and [001] and between the nodes of the directions [101] and [203] were measured at the temperatures: 240 K, 210 K, 203 K, 180 K, and 10 K corresponding to different structural phase states in the crystal. At these temperatures in addition to basic

(commensurable) peaks, satellites with the modulation wave vector **q**=(δ, σ, 0.25) were observed. It appears that the parameters δ and σ depend essentially on the temperature. For example, at T=203 K they turn into zero. The character of changes in the absolute and relative intensities of basic reflexes and satellites points to quasicontinuous changes of the $TlInS_2$ structure.

In the year 2000 a large volume of work in applied materials science was done using the neutron difffraction method. This includes many experiments to determine internal stresses in large-volume industrial products and materials, investigations of nanocrystalline objects, and studies of the texture of minerals. For example, it is shown that marbles possess clear preferred orientations with a much higher degree of the preferred lattice orientation as in dynamically recrystallized carbonate rocks. Hence, it is assumed that the behavior of samples is highly anisotropic at thermal dilatation. This is of interest from the viewpoint of machining and restoration of construction marble materials. In fact, the modeled thermal expansion coefficient α shows a pronounced anisotropy. It is concluded that knowing the texture is a must for the correct determination of the dilatation behavior of marbles (a collaboration with the Institute of Geology and Dynamics of the Lithosphere, Goettingen).

An attempt has been made to determine structural and textural changes of calcite as a function of temperature, mechanical stresses, and time under load. It is confirmed that texture changes due to directed strain and heating up to 250°C are quite small. In contrast, distinct texture changes are observed after a long time under load (20 weeks) at room temperature, which must be attributed to recrystallization processes. It is also shown that the thermal expansion coefficient of calcite α can be determined by neutron diffraction from polycrystalline samples. P-wave velocity measurements in the axial direction of the sample were used to calculate the macroscopic elastic module *E* of the sample and estimate lattice stresses.

Small-angle scattering. The scientific program for YuMO included many directions of condensed matter physics, biophysics and molecular biology, and the physics/chemistry of surfactants, colloids, and polymers, etc. The dependence of the structure and properties of TTABr micelles on the pressure and temperature were studied. It is found that in self-organizing TTABr systems an increase in the salt concentration leads to the phase transition from the ball-like to cylindrical shape of the micelles and to the growth of the radius and length of the cylinder. Increasing temperature produces the opposite effect, the radius and length of cylindrical micelles decrease.

The structure of monoglycerides widely used as emulsifiers and initiators of crystallization of water dissolved fats in food industry is studied. It is determined in what conditions monoglycerides solidification in water occurs, i.e. the gel-phase is formed, and how the formation of a homogeneous monoglyceride-water medium induced by added charged amphifills goes.

Gels and water solutions of N-vinylcaprolactam in heavy water in the presence of ionogenic surface-active substances and pyragallol are studied by small-angle scattering at different temperatures. It is shown that an addition of a thermo-sensitive polymer of different low-molecular substances may affect essentially the temperature behavior and conformation of macromolecules in the polymer.

Polarized neutrons and neutron optics. On the spectrometer SPN experiments to investigate the formation of a field of neutron standing waves in layered nanostructures and the channeling effect of neutron waves in layered structures continued. The prospective applications of these new effects may be the creation of a neutron beam with a super-narrow cross section (100 nm in diameter), formation of extramonochromatic and extracollimated neutron beams, and the use of layered neutron resonators as phase-shifting elements in spin-echo neutron spectrometers. The neutron wave channeling effect was observed in the Cu(30nm)/Ti(150nm)/Cu(100nm) structure deposited on glass. For the neutron moment transfer values 0.997, 0.0134, and 0.0182 $Å^{-1}$ the intensity peaks corresponding to an increase in the neutron density due to coherent summation of waves with different multiplicities of reflection from copper layers. It has thus been shown experimentally that neutron waves are channeled at distances larger than 30 mm. detectable off-specular scattering due to interface roughness is registered for samples with «atomic flat «

interfaces. Thus, magnetic pure spin-flip off-specular scattering can be attributed to the structure of magnetic correlations. These data are quantitatively described within the supermatrix formalism developed for the model of column-like antiferromagnetic domains (**Fig.3**). The reflection and

a)

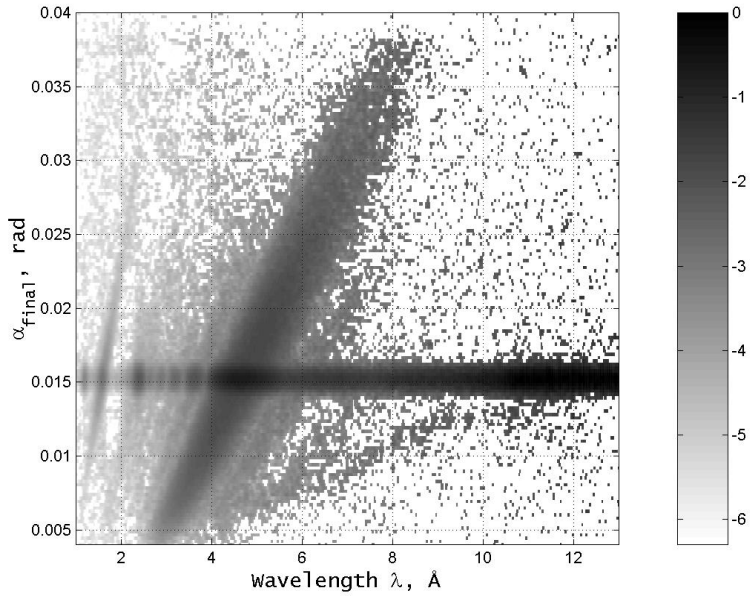

Fig.3. *a) The intensity map of the specular and off-specular scattered neutrons (spin-down) on the Fe/Cr multilayer at H=0.428 kG as a function of li and* aa_f*, the neutron wavelength and outgoing scattering angles, respectively; the incident angle* a_i *= 15 mrad;*

b)

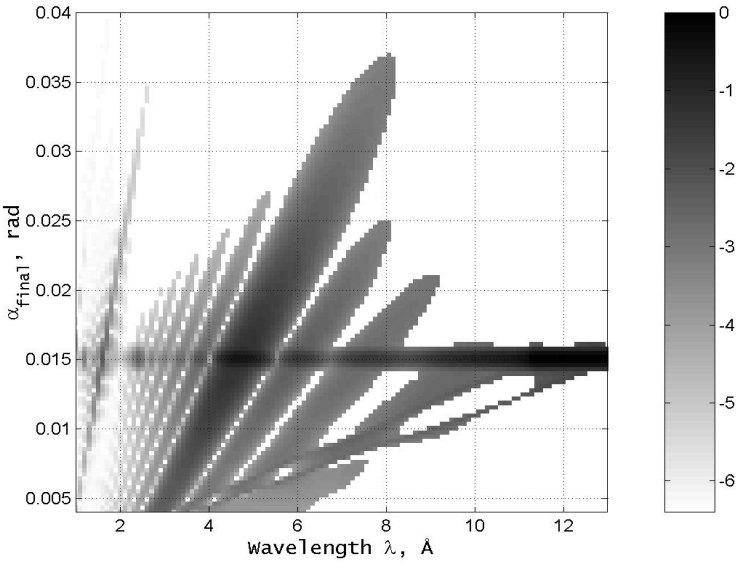

Fig.3. *b) the result of the supermatrix calculation within the model of noncollinear domains.*

polarized neutron off-specular scattering together with a complete data-analysis have been employed to verify atomic spin correlations in Fe/Cr multilayers, a typical system

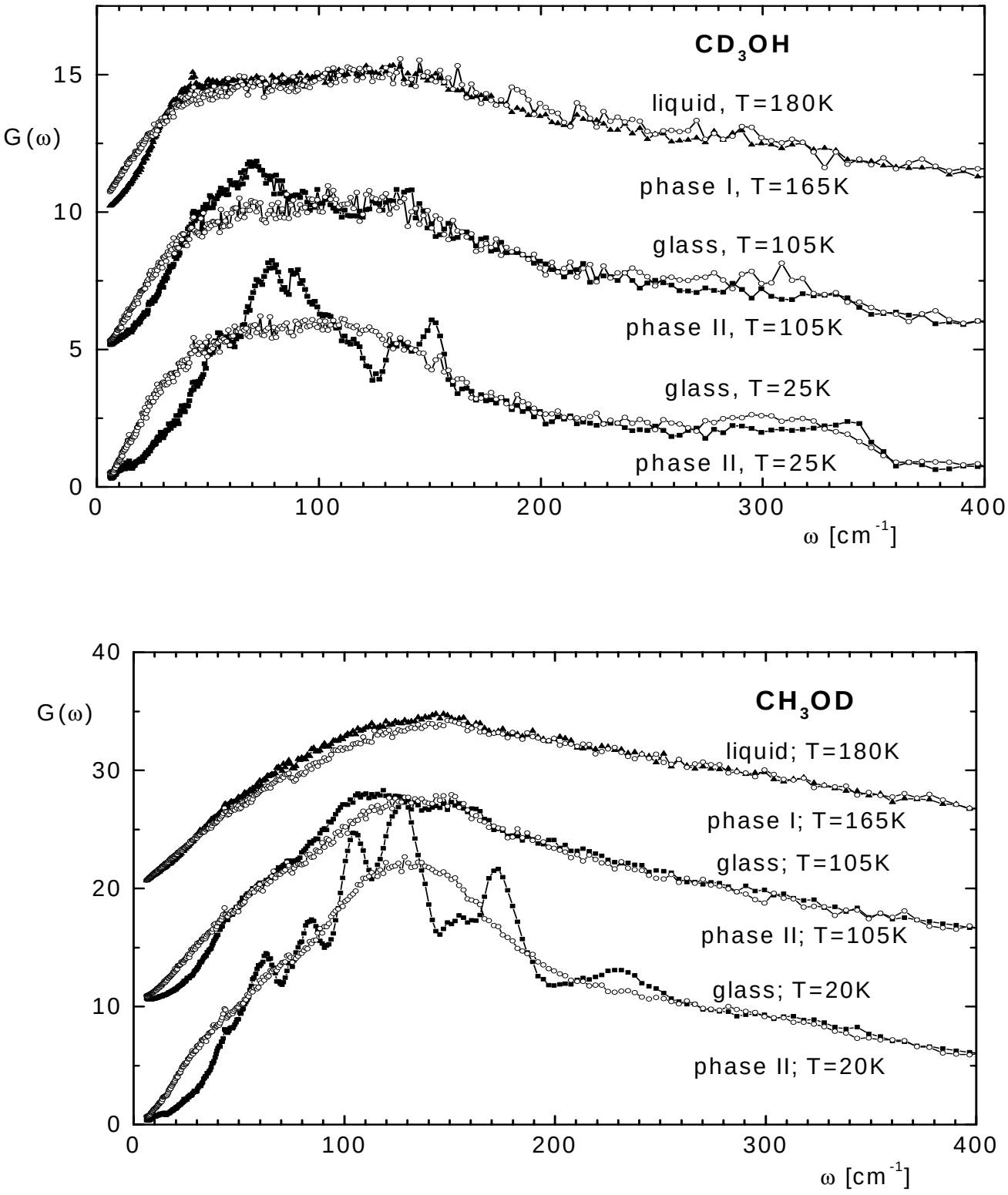

Fig.4. *The temperature dependence of the neutron scattering weighed vibrational spectra of crystalline (full square – phase II, and triangles – phase I), glassy, and liquid (open circles) methanol with partially deuterated subunits.*

showing the GMR-effect. Polarization analysis yields an important result indicating that in-plane magnetisation breaks into rather small column-like domains. For increasing external magnetic fields, within the domains spins in successive Fe-layers have an antiferromagnetic component which tends to zero along with the coupling angle. At the same time, the domain size increases. Within each domain correlations extend through the entire depth of the multilayer. No evolution of the magnetization arrangement in the range of spin-reorientation towards saturation is discussed in view of the nature of the GMR-effect. It is argued that domains may provide an efficient spin-flip mechanism for electron spin-flip scattering - a crucial ingredient of the GMR-effect.

In the spectrometer REFLEX-P-based investigations of thin polycrystalline FeCo-films indications of inelastic neutron scattering into the range of small angles are obtained, which makes it possible to assume the existence of surface or planar magnons in such substances.

Inelastic neutron scattering. On the spectrometers DIN-2PI, KDSOG-M, and NERA-PR investigations of the dynamic properties and phase transitions of metallic, molecular, and ion-molecular compounds were conducted. Most interesting NERA-PR-aided results were obtained in investigations of the dynamic disorder and glass-like phases in solid solutions and compounds containing molecular groups of the type CH_3, CH_4, H_2O or OH. The investigations were traditionally done in collaboration with scientists from Poland and Russia. In the year 2000 in the framework of this theme partial spectra of the density of vibrational states of crystalline or glass-like methanol were determined, the experiments being carried out using selectively deuterated samples of CD_3OH and CH_3OD (**Fig.4**). The obtained data were used to verify the dynamics models of the crystalline and glass-like phases of methanol and also, to determine the microscopic mechanism of arising of the «boson peak» in the low-frequency oscillation spectrum of molecular glass.

In DIN-2PI investigations of water solutions the effect of the dissolved particles on the microdynamics of water molecules entering into their hydrate spheres was determined. The effects of hydrophobic hydration and their influence on the diffuse mobility and rotation-oscillation dynamics of the hydration water molecules were studied. A comparative analysis of two types of hydration reveals the fact that large apolar particles do not destroy the network of hydrogen bonds in the surrounding water.

Investigations of the atomic dynamics of liquid metals and the behavior of impurities in them continued. Studies of Pb-K melts as prospective coolants in fast nuclear reactors of the next generation started. A DIN-2PI diffraction experiment to study a Pb-K melt with a eutectic concentration (9% at. of K) was prepared and performed. An analysis of the structure factor obtained for the region of small neutron momentum transfer reveals the absence of clasterization in this alloy in contrast to what is expected for the eutectic potassium concentration.

Investigations of the structure and dynamic peculiarities of liquids comprising laser-active systems continued. An analysis of the experimental data for liquid phosphorus oxychloride ($POCl_3$) is completed and the information inferred summarized. A search of connections between the microdynamic properties and electron excitation characteristics in this liquid was carried out. Investigations of quantum effects in restricted geometry systems continued. An experiment to study multilayer films of liquid helium on a silica aerogel was prepared and performed. The excitation spectra of liquid helium multilayer films on a silica aerogel at 1.55 K were measured for different thicknesses of helium films (see Experimental Reports).