11.8-06 MULTIPLE DIFFRACTION IN GARNETS. M.G.Shumsky, Yu.A.Rosenberg, L.I.Kleschinsky, V.M.Kiselev, A.I.Kolosovsky, I.L.Feldman, Phys. Dept., Institute of Transport's Engineers, Irkutsk 664028, U.S.S.R.

Renninger effect was studied in different crystals of garnets (AYG, GGG). It is shown that space group of investigated garnets is Ia3d not $R\bar{3}$ as previously reported (J.Chenavas et al., Journal of the Less-Common Metals 62, 373 (1978)). Appearance of the forbidden (200) and (222) reflections as J.Chenavas et al. pointed out is explained by disregard of Umweganregung peaks rise. Regularities of many-beam diffraction in garnets are discussed.

11.8-07 X-RAY DIFFRACTION FROM FCC CRYSTALS CONTAINING A NON-RANDOM DISTRIBUTION OF DEFORMATION FAULTS. By S. Lele, Department of Metallurgical Engineering, Banaras Hindu University, Varanasi 221005, India, and Dhananjai Pandey, School of Materials Science & Technology, Banaras Hindu University, Varanasi 221005, India.

In developing the theory of X-ray diffraction from faulted fcc crystals it is normally assumed that the faults are distributed entirely at random. This assumption breaks down in crystals undergoing the fcc to hcp transformation since the transformation is believed to occur through a non-random insertion of deformation faults on alternate 111 planes. The purpose of the present investigation is to develop the theory of X-ray diffraction for such crystals. For this, we have assumed that once a fault has occurred on a particular layer, it will not occur again on the very next layer. Using this model we have performed a detailed mathematical calculation to obtain an exact expression for the diffracted intensity and to predict theoretically the observable diffraction effects such as change in the intensity, broadening and the shift in the peak positions of different reflections with h-k ≠ 0 mod 3. A comparison of the theoretically predicted diffraction effects with those actually observed can enable one to establish the mechanism of transformation in materials like Co and its alloys.

11.9-01 DETERMINATION OF THE ANION POSITION PARAMETER IN MnF_2 FROM γ-RAY DIFFRACTION. By W. Jauch and J.R. Schneider, Hahn-Meitner-Institut für Kernforschung, Berlin, FRG

γ-radiation (λ = 0.0301 Å) was used to collect selected Bragg diffraction intensities on an absolute scale from a single crystal plate of rutile-type MnF_2. The objective was to detect whether there is a magnetostrictive change in the positional parameter u. The reflections were chosen for maximum sensitivity with respect to this parameter. Each reflection was measured repeatedly in order to test for multiple scattering and inhomogeneities in the mosaic structure.

Structure refinement with anisotropic temperature factors, based on 25 observations of average precision $\overline{\sigma(F_o)/F_o}$ = 0.004, yielded at room-temperature: u = 0.30530(7); $\sum w(F_o-F_c)^2/(25-8)$ = 1.05. The weights were derived from counting statistics alone. No extinction correction has been applied.

The result of diffraction measurements below the Néel-Temperature (T_N = 67 K) will be reported.

11.9-02 THEORY OF MÖSSBAUER DIFFRACTION IN MOSAIC CRYSTALS. By E.V.Smirnov & V.A.Belyakov, All-Union Research Institute of Physical-Technical & Radiotechnical Measurements, Moscow, U.S.S.R.

The theoretical investigation of Mössbauer gamma-ray diffraction in mosaic magnetically-ordered crystals based on the transport equations is presented. The equations have the following form

$$\gamma_1 \frac{d\hat{J}_1}{dz} = (\hat{A}_1 - \hat{B}_1)\hat{J}_1 + \hat{C}_{12}\hat{J}_2$$
$$\gamma_2 \frac{d\hat{J}_2}{dz} = (\hat{A}_2 - \hat{B}_2)\hat{J}_2 + \hat{C}_{21}\hat{J}_1 \qquad \text{(I)}$$

where $\hat{J}_1$ and $\hat{J}_2$ are the polarization tensors of direct and diffracted beams, $J_\rho^{i\kappa} = E_\rho^i E_\rho^{\kappa *}$, E_ρ, γ_ρ are amplitudes and direction cosines of the waves respectively, indexes $i,\kappa = 1,2$ label polarization of the waves, $\hat{A}$, $\hat{B}$, $\hat{C}$ are the matrix operators with elements depending on the structure amplitude $F_{\vec{h}-\vec{m}}^{i\kappa}$. In the limit of the nuclear resonant scattering amplitudes equal to zero the system (I) coincides with the corresponding system for X-ray diffraction (Dmitrienko & Belyakov, Acta Cryst. (1980) A36, 1044).

It is shown that the system (I) describes the dependence of intensity and polarization characteristics of diffracted beams and in particular their depolarization, on details of mosaic structure of crystal.

Two cases in which the system (I) has an

analytical solution are examined: a) the case of mutually orthogonal eigen polarizations and b) the case of high resonant gamma-ray absorption. For these cases the boundary-value problem for a crystal in the form of the plane-parallel plate is solved and analytical expressions for intensity and polarization characteristics of diffracted beams are obtained.

The case of high resonant absorption (absorption length is much smaller than extinction length) is examined in details. In this case the polarization tensor of diffracted wave may be presented in the following form

$$J_2^{ik} = \sum_{\ell,m} \frac{C_{21}^{ik\ell m} J_1^{\ell m}_{ext}}{A_2^{ikik} - \frac{\gamma_2}{\gamma_1} A_1^{\ell m \ell m}} \left[\left(1 + \frac{L}{\gamma_1} B_1^{\ell m \ell m}\right) \times \right.$$

$$\left. e^{-\frac{A_1^{\ell m \ell m} L}{\gamma_1}} - \left(1 + \frac{L}{\gamma_2} B_2^{ikik}\right) e^{-\frac{A_2^{ikik} L}{\gamma_2}} \right] \qquad (2)$$

where $J_{1\,ext}^{\ell m}$ is the polarization tensor of the incident wave, L is the crystal thickness.

Comparison of the developed approach with the results of kinematical (Belyakov & Bokun, Acta Cryst.(1975) A31, 737) and dynamical (Smirnov & Belyakov, ZhETF (1980) 79, 883) theory is carried out. It is noted that the comparison of experimental data with the calculation in framework of the presented approach may be used for estimates of crystal perfectness.

11.9-03 **DETERMINATION OF FERROMAGNETIC DOMAIN STRUCTURE BY MEANS OF MÖSSBAUER DIFFRACTION.** By R. Ch. Bokun. All - Union Research Institute of Physical-Technical and Radiotechnical Measurements, Moscow, USSR.

The new neutron methods used for examination of magnetic domains in the crystalline volume (Somenkov V.A.et al.; Schlenker M.et al.(1972-1977)) require of unique equipment and rather large specimen thicknesses>100mkm. As it will shown below,The Mössbauer diffraction of γ-quanta is usable for the less thicknesses of the magnetic crystals containing the isotope ^{57}Fe.

Mössbauer diffraction by ferromagnetic plane-bounded crystal was considered in symmetric Bragg case. The simplifying assumptions were following;the crystalline plate is divided along its thickness into two 180° domains, which are magnetized parallel to the plate boundary and to domain wall; there is the mosaic crystal with I atom Fe per cell; Rayleigh scattering at the Bragg angle is negligible; incident γ-quanta are unpolarized.Mössbauer diffraction theory for mosaic crystals was applied here. Mössbauer spectrum $I_t(E)$of Bragg reflection at an angle θ_B was calculated in the case of individual Zeeman transition with $\Delta M \neq 0$(E is a deviation of γ-quantum energy from resonant one). The certain γ-quantum polarisation distinguishing in different domains is not scattered by ^{57}Fe-nuclei. As a result the intensity $I_t(E)$ depends on a depth $t \cdot \sin\theta_B$ of the domain wall location. The effect of domain presence $W_t(E) = [I_t(E) - I^0(E)] / I^0(E)$, where $I^0(E)$ is Mössbauer spectrum in a single domain case, is given by $W_t(E) = \Psi_1^n \exp(-2\mu_R t) \cdot [1 - \exp(-\mu t y_E)] \cdot [1 + \Psi_2^n \exp(-\mu t y_E)]$, where $\Psi_{n=1;2} = (\cos^n\psi + \cos^{-n}\psi)/2$, ψ-an angle between ferromagnetic axis and the incidence direction; $y_E = (1+\cos^2\psi) / [1 + (2E/\Gamma)^2]$, Γ - the intrinsic Mössbauer line width; μ , μ_R-absorption factors for the nuclear and Rayleigh scatterings (the nuclear absorption is strong so in this case the plate thickness is accepted infinite here). For the 100% isotope ^{57}Fe crystal possessing $t<30$ mkm the maximal effect W_t exceed 5% that is quite measurable. For the determination of a depth $t \cdot \sin\theta_B$ it can be used both the dependences of intensity (or W_t): on E and on ψ. At the same time the polarization measurements of scattered γ-quanta can be used too.

11.9-04 HIGH RESOLUTION DIFFUSE X-RAY SCATTERING STUDIES OF COPPER SINGLE CRYSTALS. By Krishan Lal and Bhanu Pratap Singh, National Physical Laboratory, Hillside Road, New Delhi - 110012, INDIA.

In the melt grown crystals at the growth temperature the concentration of vacancies is very high. As the crystal is cooled to room temperature all the vacancies in excess of the thermodynamically expected number are unable to move out of it. In the present investigation these excess vacancies and their aggregates have been studied by measuring diffuse X-ray scattering (DXS). The following two types of crystals have been investigated: (1) As grown crystals (Sample A), (2) Crystals which have been subjected to prolonged annealing near melting point to reduce the concentration of excess vacancies (Sample B). DXS measurements have been made on a triple crystal X-ray diffractometer around 200 reciprocal lattice point (relp) with the scattering vector along the reciprocal lattice vector, perpendicular to it and at 45° to it. The distribution of the DXS intensity around the relp is very different in Sample A from that in Sample B. This shows that as in the case of Si single crystals (Lal and Singh, Acta Cryst. A36, 178 (1980)) and alkali halide single crystals (Lal and Singh, ICCG-VI, Moscow, (1980)), in Cu also the main contribution to the observed DXS is from defects present in the specimen. There is no significant contribution from phonons at room temperature. Mainly vacancy type defects are present. Vacancies are observed to cluster in Sample B. Detailed study of the size and shape of the vacancy clusters is made.