Extinction in real crystals is understood as the violation of the kinematic relation

$$\rho = \lambda^3 \cdot |F_G|^2 \cdot V/(\Omega \sin 2\theta_B) = Q \cdot V \qquad (2)$$

between the integrated reflecting power and crystal volume. This can occure in two ways:

A - proportionality between ρ and V is conserved, but with a different constant $q < Q$; this effect, being independent of the total crystal volume, is to be atributed to interference of coherent waves scattered by neighbouring atoms
B - gradual saturation of (2) starts above some value V_o, being caused by multiple reflections on equally oriented crystallites; as a consequence of the statistical nature of the mosaic structure a sufficiently long beam path in the crystal is necessary to provide appreciable probability of this effect; the small neutron coherence length ($\sim$3 nm) in usual experiments implies the incoherent nature of this process.

Based on this argumentation the following improvement of the existing extinction theory is proposed: The primary extinction should be identified with the A mechanism and described by a mean value of the reflectivity P(Θ) given by eq.(1). The conventional treatment (Becker and Coppens, Acta Cryst. A30(1974)129) based on the intensity-coupling equations with accordingly modified coefficients should be used for secondary extinction (B) only, where its use seems fully justified from the physical point of view.

problem of the MLC-structure reconstruction within the framework above mentioned MLC-models. It is shown, that the inverse problem of the MLC-structure reconstruction has a unique solution. We believe, that the earlier in (*, **) developed characteristic matrix method makes it possible to optimize the number of fitting parameters and to reduce the diffractional problem to the solution of some recurrence equations for amplitude reflection R^g and transmission T^g coefficients (ARC and ATC, correspondingly). Accordingly to (**) the recurrence formulae are given by

$$R_n^g = R_1^g + R_{n-1}^g T_1^g T_1^{-g}(1 - R^{-g} R_{n-1}^g)^{-1},$$

$$T_n^g = T_1^g T_{n-1}^g (1 - R_1^{-g} R_{n-1}^g)^{-1},$$

where R_1^g and T_1^g are ARC and ATC for the first layer and R_{n-1}^g, T_{n-1}^g for remaining n - 1 layers in total. The coefficients R_{n-1}^g and T_{n-1}^g are determined in the same way and so on. In the particular case $R_i = r$ and $T_i = t$ (i = 1, ...,n) the recurrence formulae give ARC and ATC for dynamical diffraction in a superlattice. In conclusion we give some concrete examples of the semiconductor thin films structure reconstruction on the symmetrical Bragg diffraction data basis. Treating this as an inverse problem of the X-ray diffraction, we have determined the film thickness, lattice parameter distortion and components concentration from the entrance surface deep into the film. We discuss the internal stress influence too.

11.7–14 X-RAY DIFFRACTION IN MULTILAYER CRYSTALS (MLC). By A.V.Kolpakov, Department of Physics,Moscow State University, Moscow, USSR.

In the report are discussed possibilities of MLC-investigations by X-ray diffraction and offered a critical analysis of the appropriate theoretical and experimental results. The relevant MLC-structures are: heteroepitaxial films, heterojunctions, superlattices, ion implanted surface layers and so on. All mentioned objects have onedimensional layerlake structure due to smooth or stepwise varying lattice parameter. The ground problem is how to get to know the MLC-structure without destroing it. The MLC are usually from 10 Å up to 10^5 Å thick. Such MLC can be investigated in this thickness range only through X-ray diffraction. The analytical solutions of the diffraction problem in kinematical and dynamical approximations were obtaind up to day for some ground MLC-models only: for a crystal with a constant deformation gradient (Chukhovskii F. N. Metallofizika, 1981, No 3, 5; Khapachev Yu. P., Kolpakov A.V. et al. Vestn. MU, ser. No 3, 1980, 21, No 5, 57); superlattices (Kolpakov A.V., Khapachev Yu.P. Kristallografija, 1973, 18, No 3, 474); step functions (Petrashen'P.V. Fizika tverdogo tela, 1975, 17, No 9, 2814; Kolpakov A.V., Belyaev Yu.N. Dep. v VINITI, No 3334-81, Dep. (*)). On the basis of the analytical solution of the direct problem X-ray diffraction in a steplike crystal the reconstruction methods of such crystal structure are developed (Afanasev A.M. et al. phys. stat solidi (a), 1977, 42, 415; Belyaev Yu. N.,Kolpakov A.V. ibid., 1983, 76, 641 (**)).
We treat with a formulation of the inverse

11.7–15 THE RECONSTRUCTION OF THE MULTILAYER CRYSTAL (MLC) STRUCTURE FROM X-RAY DATA AS AN INVERSE PROBLEM (IP). By A.V. Goncharskii and A.V.Kolpakov, Department of Physics, Moscow State University, Moscow, USSR.

The X-ray diffraction direct problems (DP) have been analytically treated for some simple models, which describe onedimensional lattice constant variations in such important from practical point of view objects as heteroepitaxial thin films, heterojunctions, superlattices and ion implanted surface layers (see e.g.: Chukhovskii F.N. Metallofizika, 1981, 3, No 5, 3 (*);Kolpakov A.V. et al. Kristallografija, 1977, 22, 437; Khapachev Yu.P. et al. ibid., 1979,24, 430; Afanasev A.M. et al. phys. stat.sol. (a), 1977, 42, 415; Belyaev Yu.N., Kolpakov A.V. ibid., 1983, 76, 641).
We report about formulation IP of the reconstruction MLC-structure from X-ray diffraction data. This formulation is based on the DP $f = Az$ solution (z - MLC-characteristics, f - - input information parameters). The theoretical spectrum $f^T(\vartheta)$ (ϑ - scattering angle) is a convolution integral of the DP solution $g(\vartheta)$ and the apparatus function $K(\vartheta - \vartheta')$, which is a priori known or may be defined from IP-solution. We take as an example the symmetrical Bragg diffraction in a crystal plate, which has a finite thickness. The crystal lattice has a linear onedimensional lattice constant variation. Further we make use of the recently received analytical solution this problem (Kolpakov A.V., Punegov V.I., to be published). We introduce and analyse the random value $\Delta(\vec{a})$. The dimensionality of the vector $\vec{a}$ equals of the MLC-parameters number (i.e. thickness t ,