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

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

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_0, being caused by multiple refledtions 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 $P(\theta)$ 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.

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 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

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

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

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.

11.7–15 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 $\Delta(\vec{\alpha})$. The dimensionality of the vector $\vec{\alpha}$ equals of the MLC-parameters number (i.e. thickness t ,

chahge in the interplanar spacings $\Delta d/d$, $d(x)$ and so on). The $\Delta(\vec{a})$ is distributed to Fisher. The $\Delta(\vec{a})$ is defined by the expression:

$$\Delta(\vec{a})=\frac{N-M}{M-1}\sum_{K=1}^{M} N_K f_K^{-1}\left(\bar{\xi}_K-\hat{c}\,f^T(\vartheta_K,\vec{a})\right)^2 \Big/ \sum_{K,j=1}^{M,N_K} f_K^{-1}\left(\xi_K^j-\bar{\xi}_K\right)^2,$$

where $N=\sum_{K=1}^{M} N_K$ – a full number of measurements, $\hat{c}$ – parameters c value, that minimizes the quadratic form $S(c)=\sum_{K=1}^{M}\frac{N_K}{f_K}\left(\bar{\xi}_K-c\,f^T(\vartheta_K,\vec{a})\right)^2$, for any ϑ_K : N_K – number of measurements, ξ_K^j – result of the j-th measurement, $f_K\sigma^2$ – – dispersion of measurements error, σ^2 – unknown parameter, f_K – an unknown true value of measurement, which can be good estimate by the mean value $\bar{\xi}_K=\sum_{j=1}^{N_K}\xi_K^j\cdot N_K^{-1}$, $f^T(\vartheta_K,\vec{a})$ – is a theoretical value for the fixed vector $\vec{a}$. We analise the confidens set $\mathbb{D}$, whose elements are vectors $\vec{a}$, for which take place inequality $\Delta(\vec{a})\leq F_{M-1,N-M,\alpha}$ (α – the given confidence level). The problem of the confidence intervals construction can be solved by the simple sorting of the vectors $\vec{a}$ values near $\vec{a}_{min}$, which minimizes $\Delta(\vec{a})$. For a small number of the model parameters the problem is stable. When the number is large, it is necessary to make use of the regularizating algorithms (Tikhonov A.N. et al. Regulariziruju - shtchije algoritmy i apriornaja informatsija. Moscow, Nauka PH, 1983, p.195).

11.7–16 EFFECTS OF WEAKLY EXCITED REFLECTIONS ON THE TWO-BEAM CASE OF DYNAMICAL X-RAY DIFFRACTION. By H. K. Wagenfeld, Royal Melbourne Inst. of Technology, Melbourne, Australia, and H. J. Juretschke, Polytechnic Inst. of New York, New York, USA.

Bethe(1928, Ann. Phys.,Lpz. 87,55) formulated the dynamical theory of electron diffraction for a two-beam case and included weakly excited additional reflections by adding perturbation terms in the potential. A systematic extension of this method to x-rays,including coupling of the two polarizations (Juretschke, 1984, Acta Cryst., to be published) can be used to predict changes in two-beam properties caused by additional reflections, for Laue and Bragg cases. Hart and Lang (1961, Phys. Rev. Lett. 7,120) showed that Pendellosung fringe spacings are changed to an Aufhellung by the excitation of extra reflections. This change in spacing follows directly from the changes in effective structure factor and in the absorption coefficient of the standard two-beam interaction predicted by the theory for this four-beam case.

11.7–17 X-RAY STANDING WAVE MEASUREMENTS OF NONCENTROSYMMETRIC STRUCTURES) By M. Bedzyk and G. Materlik, Hamburger Synchrotronstrahlungslabor HASYLAB, Hamburg, Germany.

When diffracting an x-ray plane wave from a single crystal, the diffracted and incident traveling plane waves interfere to form a standing wave-field. As is known, the phase of this interference pattern relative to the diffraction planes is a function of the Bragg reflection angle.
For a noncentrosymmetric Bragg reflection from a III-V single crystal, the position of the diffraction planes relative to the atomic lattice depends on the x-ray scattering factors $f(\bar{H})$ of the two different atomic species. Due to anomalous dispersion, this diffraction plane position is in turn dependent on the x-ray energy. As an example, with respect to the corresponding centrosymmetric position, the (111) noncentrosymmetric diffraction planes are shifted in the $[\bar{1}\bar{1}\bar{1}]$ direction by an amount:

$$\Delta(111) = -\frac{1}{8} + \frac{1}{4\pi}\left[\tan^{-1}\left(\frac{f_V^0+f_V'+f_{III}''}{f_{III}^0+f_{III}'-f_V''}\right)+\tan^{-1}\left(\frac{f_V^0+f_V'-f_{III}''}{f_{III}^0+f_{III}'+f_V''}\right)\right],$$

where $f=f^0+f'+if''$. (f' and f'' are the anomalous dispersion corrections.) In an x-ray standing wave measurement the position, of either one of these two atoms, relative to the diffraction planes can be determined and used to calculate the noncentrosymmetric shift $\Delta(\bar{H})$. By using the energy tunability of the x-ray standing wave instrument installed at the Hamburger Synchrotron Radiation Laboratory, it was possible to measure the energy dependence of $\Delta(111)$ in the vicinity of the respective K absorption edges for a GaAs(111) single crystal.

11.7–18 POLARIZATION-MIXING OF X-RAYS (QUANTUM THEORY OF INTERFERENCE OF WHITE X-RAYS). By T.Ohkawa and H.Hashimoto*), The Institute of Vocational Training,Sagamihara city,Kanagawa, Japan,*) Department of Applied Physics, Osaka University, Suita, Osaka, Japan.

X-ray polarization effect has been a vexing problem which has recently been given serious interest, however conventional theoretical predictions have failed to explaine the origin of the rotation of polarization direction. In order to sutdy the mechanism of the polarization of x-rays in crystal, relativistic quantum field theory is applied to the process of x-ray diffraction. Two photon state is theoretically investigated for analysing the mechanism of the polarization-mixing. This theoretical method is also applicable to discuss the resonative interference of white x-rays of proximate energy. The Feynman's graphical method is employed to expand the 2nd order perturebation, in which inner photon-line of quantum theoretical concept is introduced which is assumed to have analogical meaning to Ewald's "Winnen Welle" that traveles in the crystal field with radiationless dipolewave. The conventional structure factor has been expanded with static electron's distribution, however to discuss the interference phenomena taking place in atomic field, dynamic nature of electron's behaviour is necessary to incorporate, so that dispersion relation of diffracted x-rays similar to Laue's dynamical theory is shown by use of scattering S-matrix. Dynamical structure factor is defined on the base of Dirac's matrix.