11.7–11 EXPERIMENTAL DETERMINATION OF ENANTIOMORPHS BY THREE-BEAM DIFFRACTION.
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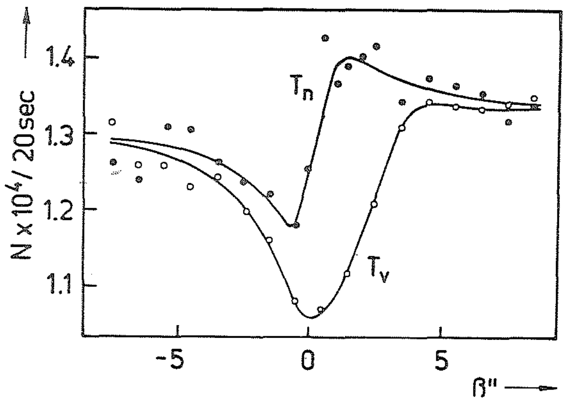
The experimental determination of structure invariant triplet phases allows the fixing of the absolute configuration. By recent investigations it is well established that the triplet phase sum Φ of F(-h)F(g)F(h-g) can be deduced from the rocking curve profile of a Psi-scan experiment scanning trough a three-beam position. For non-centrosymmetric structures four typical profiles can be observed. For $\Phi=0, \pi$ asymmetric profiles result, whereas $\Phi=\pm\pi/2$ result in a symmetrical decrease or a symmetrical increase respectively.
In a first approximation this behaviour can be explained by the superposition of the wave diffracted by the net planes of h and the "Umweg" wave successively diffracted by the net planes of g and h-g. Their phase relationship is governed by the constant triplet phase and an additional resonance phase shift by π, caused by the reciprocal lattice vector g passing through the Ewald sphere. Simultaneously the amplitude of the "Umweg" wave is turned on and off continuously. The interference between both waves can be graphically displayed by a vector diagram in the complex plane.
As the triplet phases of enantiomorphs differ in the sign of their imaginary parts in this case highest influence to the Psi-scan profiles is for $\Phi=\pm\pi/2$ and the two cases can be well distinguished. Experimental results of L-Asparagine will be reported.

11.7–12 CONTROL OF ANOMALOUS NEUTRON TRANSMISSION BY ULTRASONIC VIBRATIONS.
By B. Chalupa, R. Michalec and P. Mikula, Nuclear Physics Institute, Czechoslovak Academy of Sciences, 250 68 Řež near Prague, Czechoslovakia.

One of the most important phenomena following from the dynamical diffraction theory is the effect of anomalous transmission (AT) of radiation (X-rays, neutrons) through absorbing perfect crystal (G. Borrmann, Z. Phys.(1941) 42 157; D. Sippel, Phys. Lett. (1964) 8, 241). Deviations from the ideal structure (imperfections, elastic deformation) bring about the distortion of the wave field inside the crystal and partially or completly restore high absorption.
The effect of AT may be significantly influenced by means of ultrasonic vibrations in the crystal which may have either resonant or non-resonant character.
Ultrasonic vibrations having the wavelength equal to the extinction thickness and the wave vector parallel to $\Delta\vec{K} = \vec{K}_{01} - \vec{K}_{02}$ (perpendicular to the scattering vector) may bring about a suppression of the AT due to resonance interzonal scattering mixing Bloch states on the upper and lower branches of the dispersion surface (I. R. Entin, ZhETF Pis. Red. (1977) 26, 392; V.K. Ignatovich, R. Michalec, P4-83-189, Preprint JINR Dubna (1983).
When the vibrations are excited in the direction perpendicular to $\Delta\vec{K}$, the AT effect may be influenced through the elastic deformation caused by them. Furthermore, in case of thermal neutrons, Doppler effect may play a significant role in the studied diffraction process.

Recently we have studied the influence of mechanical resonance vibrations on AT of neutrons in a perfect InSb single crystal having the thickness t equal to 10 mm ($\mu t \approx 2\times10^2 m^{-1}$, μ - linear absorption coefficient). A double crystal (1,-1) arrangement was employed using the neutron of 0.118 nm wavelength, reflected by (220) planes. The FWHM of the double-crystal rocking curve was 1.8 seconds of arc.



The above displayed figure represents the experimentally measured transmission curves for nonvibrating crystal (T_n) and for the same crystal vibrating at a frequency of 2.26 MHz (T_v), excited into vibrations by means of piezoceramic $BaTiO_2$. The restoration of the AT effect depends on the vibration amplitude and as such may be easy controlled.

11.7–13 EXTINCTION IN NEUTRON DIFFRACTION. A QUANTUM MECHANICAL TREATMENT.
By J. Kulda, Nuclear Physics Institute, Czechoslovak Academy of Science, 250 68 Řež near Prague, Czechoslovakia.

The usual approach based on analogy with the optical treatment for X-rays is abandoned in favour of a consequent application of quantum mechanics facilitated by the completely nonrelativistic character of the neutron wave propagation. Starting from the time-dependent Schroedinger equation (SE) a unified formulation of the diffraction theory is obtained including as a limiting case the usual dynamical theory for perfect crystals based on the stationary SE.

The Takagi equations are shown to be equivalent to the time-dependent SE recorded in matrix form in the representation of the plane waves $\exp(i\vec{K}_G\vec{r})$. Their exact solution for a deformed crystal is bypassed by calculation of the probability of transitions between the neutron eigenstates caused by the time variation of the interaction potential. A simplified form of the expression for reflectivity (Kulda, Acta Cryst. A40 (1984)) is derived

$$P(\theta) = 1 - \exp(-Q|\partial\theta/\partial s_0|^{-1}) \qquad (1)$$

yielding a good approximation for a wide range of types and magnitudes of elastic deformation.

The 1st order perturbative solution of the time-dependent SE yields for the integrated reflectivity an identical formula as the kinematical approximation. The higher orders represent the contributions of multiple processes to the scattering amplitude of the crystal.

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.

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

$$R^g_n = R^g_1 + R^g_{n-1} T^g_1 T^{-g}_1 (1 - R^{-g} R^g_{n-1})^{-1},$$

$$T^g_n = T^g_1 T^g_{n-1} (1 - R^{-g}_1 R^g_{n-1})^{-1},$$

where R^g_1 and T^g_1 are ARC and ATC for the first layer and R^g_{n-1}, T^g_{n-1} for remaining n - 1 layers in total. The coefficients R^g_{n-1} and T^g_{n-1} are determined in the same way and so on. In the particular case $R_i = r$ and $T_i = t$ ($i = 1, \ldots, n$) 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 $\Delta(\vec{a})$. The dimensionality of the vector $\vec{a}$ equals of the MLC-parameters number (i.e. thickness t ,