11.7–11 EXPERIMENTAL DETERMINATION OF ENANTIOMORPHS BY THREE-BEAM DIFFRACTION.

By K. Hümmer and H. Billy, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Loewenichstr. 22, Universität Erlangen, FRG.

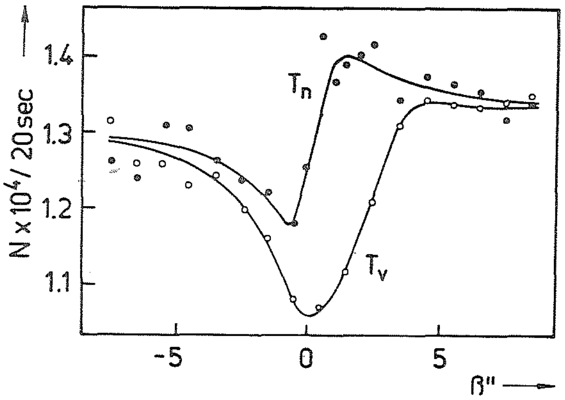
The experimental determination of structure invariant triplet phases allows the fixing of the absolute configuration. By recent investigations it is well established that the triplet phase sum Φ of $F(-\underline{h})F(\underline{g})F(\underline{h}-\underline{g})$ can be deduced from the rocking curve profile of a Psi-scan experiment scanning trough a three-beam position. For non-centrosymmetric structures four typical profiles can be observed. For $\Phi=0$, π 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 $\underline{h}$ and the "Umweg" wave successively diffracted by the net planes of $\underline{g}$ and $\underline{h}-\underline{g}$. Their phase relationship is governed by the constant triplet phase and an additional resonance phase shift by π, caused by the reciprocal lattice vector $\underline{g}$ 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 ($\mu t \approx 2x10^{2} m^{-1}$, 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.