

remarkable softness. X-ray absorption coefficients are small. The latter crystals, however, are ideally perfect. X-ray absorption coefficients are very large. TDS related to the excess line is relatively strong. The excess line across the diffuse scattering can be explained by the anomalous transmission of the TDS.

#### 11.7-2 SIMULATION OF X-RAY TRAVERSE TOPOGRAPHS

by Y. Epelboin and A. Soyer, Laboratoire de Minéralogie-Cristallographie, associé au CNRS, Université P. et M. Curie, Paris, France

The two main difficulties, to simulate the image of a defect, in a traverse topograph, are the required precision of the numerical algorithm and the time needed to integrate the Takagi-Taupin equations. The precision of varying step algorithms permits now such a calculation. However, we have found that the reciprocity theorem could not be applied to this computation because the accuracy of the algorithm is still insufficient.

Comparisons of computed profiles of intensity through the image of a dislocation with the corresponding experiment show that the simulation of the real experiment i.e. the addition of individual section topographs gives simulated images of good quality.

Since the time of computation would be too long, also when using giant computers, we wrote the program in assembler language for an array processor linked to a local small machine. The performances are very good and it has been possible to simulate images of dislocation in a reasonable time.

We have studied the influence of the Burgers vector on the contrast of dislocations and shown that it is often possible to determine both its sense and magnitude.

Our study of packets of dislocations perpendicular to the faces of a lithium formate crystal show that the image predicted by simulation of traverse topographs is quite different from the one when using the kinematical approach. It suggests that for such an orientation and for such large deformations, the image could be predicted using the criterion of the geometrical optics.

Simulation of traverse topograph can now be used for defects characterization. It might be a first approach to understand the contrast of Laue images in synchrotron experiments.

11.7-3 CIRCULAR POLARIZATION OF X-RAYS VIA BRAGG SCATTERING. By Boris W. Batterman, Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-1000 Berlin 33; and Cornell High Energy Synchrotron Source (CHESS), Cornell University, Ithaca, New York, USA..

In Bragg reflection from perfect crystals, dynamical theory predicts a  $180^\circ$  phase shift as the Darwin curve is traversed in angle-space. Indirect experimental verification of this is the motion of standing waves (Batterman, Phys. Rev. (1964) 133, A759) as an incident wave scans the range of total reflection. By combining  $\sigma$  and  $\pi$  polarization curves, relative phase shifts as large as  $50^\circ$  should be achievable experimentally. Experiments in progress will attempt to confirm that a phase shift of  $90^\circ$  (i.e., circular polarization) can be obtained. The device is the X-ray analogue of the optical Fresnel rhomb.

Research supported by a grant from the Alexander von Humboldt Foundation.

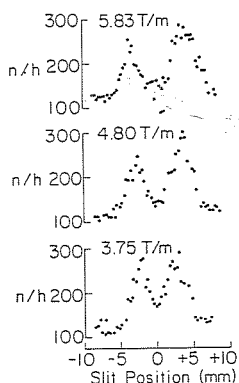
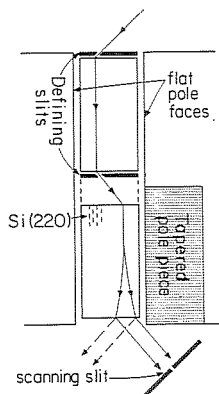
11.7-4 MEASUREMENT OF THE EFFECTIVE MASS ENHANCEMENT OF THE DEFLECTION OF NEUTRONS IN PERFECT CRYSTALS. By A. Zeilinger, C. G. Shull and M. A. Horne, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139 and S. A. Werner, Department of Physics, University of Missouri, Columbia, MO 65201 USA.

Theory predicts that neutrons propagating inside a crystal under dynamical diffraction conditions will suffer highly enhanced deflections if subject to an external force. This phenomenon is due to the large curvature of the dispersion surfaces in the vicinity of the Laue point. By analogy to the case of electrons in solids, this behavior may be interpreted as being due to an effective mass of neutrons in crystals. This effective mass is of tensor character and of positive or negative sign. Its magnitude varies with neutron propagation direction and it is smallest for neutrons propagating along the lattice planes while for neutrons propagating along the edges of the Borrmann triangle the effective mass approaches the free-space mass of the neutron.

In the experiment, neutrons of  $\lambda=2.464\text{\AA}$  were defined by a crystal collimator such that only neutrons within  $\pm 9.4 \times 10^{-8}$  radians of the chosen Bragg-angle, were passed through the system. The propagation of these neutrons in a 52.1mm thick Si-crystal set at the exact Bragg condition in Laue transmission was then studied. Without a magnetic field these neutrons were found to propagate along the (220) lattice planes as expected. A magnetic field with a gradient oriented normal to the lattice planes was then turned on in order to provide a force acting on the neutrons while propagating inside the crystal. The resulting beam deflections were found to be larger by a factor of  $2.1 \times 10^5$  than those expected in the same field gradients in vacuum. This is in agreement with theoretical prediction based on the effective mass model. Using slightly off-Bragg neutrons and studying the polarization of the resulting beams, the sign of the effective mass was experimentally determined. Again in agreement with expectation it was found that the effective mass of  $\beta$  wave field

neutrons is positive while the effective mass of a wave field neutrons is negative in the vicinity of the Laue-point, the latter wave field having its nodes at the lattice planes.

Possible applications of the low effective mass for fundamental physics studies and for neutron topography will also be discussed.



11.7-5 SOLUTION TO THE X-RAY PHASE PROBLEM FOR ACENTRIC CRYSTALS. By S.L. Chang and J. A.P. Valladares, Instituto de Física, UNICAMP, Campinas, SP, 13100, BRASIL.

An experimental method to solve the X-ray phase problem for noncentrosymmetric crystals is developed, using Bragg-type three-beam diffraction. This method results from a consideration of the phase dependence of line profiles in 3-beam reflections for wavelength  $\lambda$  above and below a critical absorption edge  $\lambda_E$  of the heaviest constituent atom in the crystal. It is found that for  $\lambda < \lambda_E$  the sign of the sine of invariant phase is a product of the signs defined from asymmetry of the line profile and the sense of rotation of the crystal lattice. Application of this method to several 3-beam cases shows an exact agreement between the experimentally determined phases and the theoretical ones. Comparison between this method and the previously proposed method for centrosymmetric crystals (Chang, Phys. Rev. Lett. 48, 163, 1982) is given. Dynamical calculation has also been carried out to provide dispersion surface and diffracted intensities for Bragg-type and transmission-type multiple diffractions in centro- and noncentro-symmetric crystals. It is shown that the phase-dependent line-profile asymmetry is an effect due to total reflection in 3-beam Bragg-type diffraction and that the line-profile asymmetry of transmission-type diffraction fails to provide correct phase information. Support from SUBIN, Telebrás, CNPq and FINEP.

11.7-6 TWO EXPERIMENTAL TECHNIQUES MEASURING X-RAY PENDELLÖSUNG INTENSITY BEATS USING WHITE RADIATION. By T. Takama, K. Kobayashi and S. Sato, Faculty of Engineering, Hokkaido University, Kita-ku, Sapporo, Japan.

A technique measuring the X-ray Pendellösung intensity beats of white radiation diffracted from perfect single crystals has been developed in the authors' laboratory. The intensity variations are directly measured with respect to the wavelength by using a solid-state detector and the energy-dispersive diffraction method. The values of the atomic scattering factors of Si, Ge, Cu, Al and Zn and their wavelength dependence have so far been determined by this technique. This method (No. 1) corresponds to the so-called "traverse topograph" taken of wedge-shaped specimen with characteristic X-rays.

A similar but slightly different method (No. 2) which corresponds to the "section topograph" was recently tried to measure the beats as well. The white radiation from a high energy X-ray generator falls upon a thick and parallel-sided perfect Si crystal in the symmetrical Laue position through a slit system. The diffracted intensities going out of the exit surface of the specimen were successively measured at the center of the Borrmann fan by changing the Bragg angle. Since the measured beats were composed not only of a large amplitude but also of a high frequency in the second method as shown in Fig. 1, the error in the obtained values of the atomic scattering factor was reduced to about one tenth of that in the first technique. See Fig. 2.

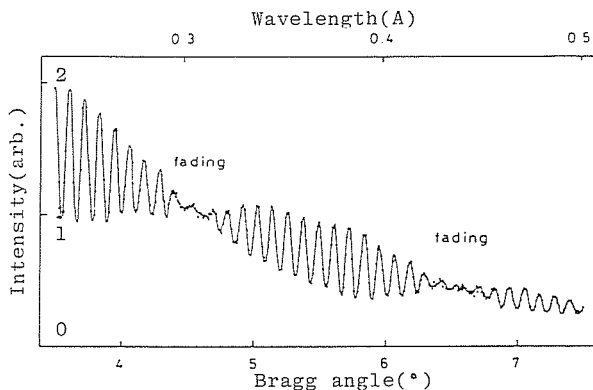


Fig.1 An example of measured Pendellösung intensity beats in the second method: Si, 220 reflection,  $t=3.478$ mm.

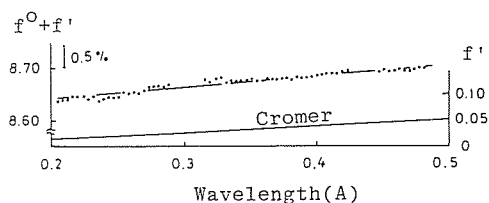


Fig.2 Atomic scattering factors,  $f^0 + f'$ , of Si obtained from the beats in Fig.1, showing a clear wavelength dependence. The dispersion term  $f'$  calculated by Cromer is also shown.