11.7–25 INFLUENCE OF MINUTE CRYSTAL STRAINFIELDS ON LAUE CASE ROCKING CURVES: A THEORETICAL STUDY.

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Laue case rocking curves of a pair of highly perfect crystals display a detailed fine structure in the low-absorption case ($\mu_0 \cdot t \leq 2$, μ_0:absorption coefficient, t: crystal thickness). The precise shape of the oscillations on the wings of the rocking curves depends very sensitively on the scattering factor of the crystal atoms, thus allowing measurements of the structure factor of silicon with uncertainties well below 0.1% (Teworte & Bonse, 1984).

In this context, the question of the influence of minute residual strain in the crystal on the shape of the rocking curve is discussed. In incident-spherical-wave approximation, beam paths and phase integrals are numerically computed on the basis of the ray optical theory in the form given by Bonse (1964). Rocking curves of pairs of crystals with built in $\frac{\Delta d}{d}$ fluctuations and local lattice rotations are presented. An example is shown in Fig. 1. The influence of strainfields on the precision of the structure factor measurements is discussed and limits of such measurements for a given crystal perfection are deduced.

References: U.Bonse, Z.Phys. 177,385(1964)
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Phys.Rev. B29,2102 (1984)

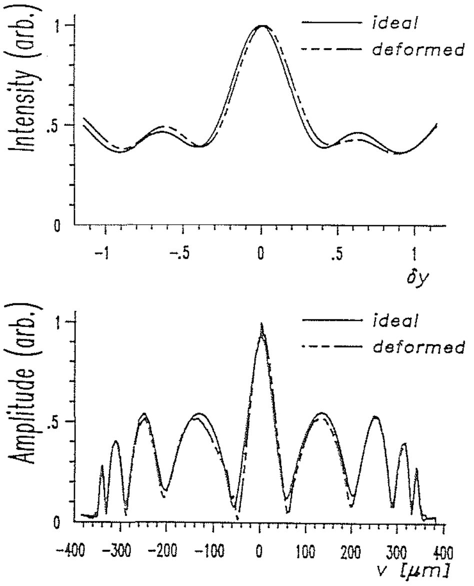

Fig.1 Rocking curve (top) and intensity distribution at the exit surface for y=0.24 (bottom) of ideal and deformed crystals. Si 555-reflection, λ=0.559 Å. Crystal thickness is 350 μm. The deformation state is given by $NN=2 \times 10^{-10} \mu m^{-1} \times \sin(0.025 \times v[\mu m])$.

11.7–26 PRIMARY EXTINCTION IN SPHERICAL CRYSTALS.

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The extinction factor appropriate to perfect crystal spheres is found to be

$$y = (1+x^2)^{-\frac{1}{2}}$$

$$x = \frac{3}{4} N_c \lambda F D$$

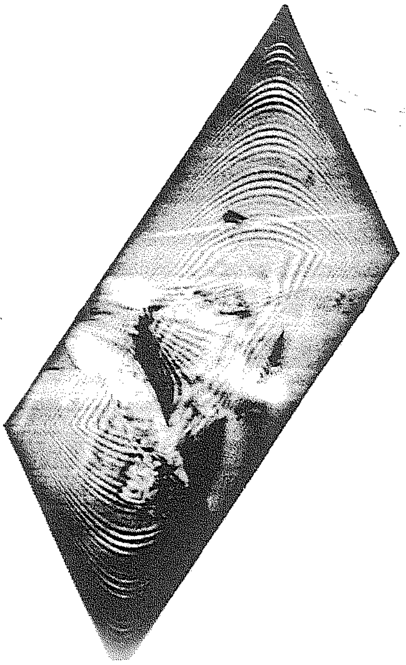
N_c = Number of unit cells per unit volume
λ = Wavelength
D = Crystal diameter
F = Structure factor per unit cell and includes the Debye-Waller factor.

Experimental tests of the validity of this expression have been made using MgO powders of controlled grain size and shape. Two diffraction geometries have been used; fixed wavelength, variable 2θ, at the HIFAR reactor and variable wavelength, fixed 2θ at IPNS. Experimental extinction factors are obtained by taking ratios of integrated intensities (assuming that extinction is negligible for grain sizes <1μm).
Theoretical extinction factors are obtained by a determination of D by scanning electron microscopy and the use of the known crystallographic parameters of MgO. There are no adjustable parameters. Theory and experiment are compared in this paper.

11.7–27 A QUANTITATIVE STUDY OF FADING PHENOMENON OF PENDELLÖSUNG FRINGES IN CRYSTALS.

By S. S. Jiang, Department of Physics, University of Nanjing, Nanjing, China.

The fading phenomenon of pendellösung fringes in diamond crystals has been studied by x-ray diffraction section topography. The fading periods of dynamical interference fringes have been observed in plate- like crystals and wedge-shaped crystals, as well as in crystals containing a stacking fault. In case of plate-like crystals, the number of fringes in each fading period observed in (1̄11̄)section topograph with Cu radiation is approximately equal to 3.08 which is what we calculated. In case of wedge-shaped crystals, the fading phenomenon of hook-shaped fringes can be seen in (2̄20) section topograph with Mo radiation (Fig.1). On the other hand, the hyperbolae of constant phase in Borrmann fan is simulated by computer according to dynamical diffraction theory, in which both π and σ polarization state are overlaped. Evidently, the number of fading period is nearly the same for both experimental results and theoretical simulation. In case of crystals containing a stacking fault, hour glass image is dominated by I_3 fringes in (1̄11̄) section topograph with Cu radiation. The fading phenomenon of I_3 fringes can be also seen, and the number of fading period is about 10.4 which is very close to the theoretical calculation 10.35. In conclusion, the quantitative comparison of experiment with theory has been made and the agreement is found to be quite good.



(Fig.1)

11.7–28 DYNAMICAL NEUTRON DIFFRACTION STUDIES ON Si SINGLE CRYSTALS BY THE TOF METHOD.

By Yu.A. Alexandrov (1), B. Chalupa (2), J. Kulda (2), T.A. Machekhina(1), R. Michalec (1), P. Mikula (2), L.N. Sedláková(1), M. Vrána (1).
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The usage of high intensity pulsed neutron sources in connection with the time-of-flight (TOF) method opens interesting possibilities in the investigation of neutron-optical phenomena such as simultaneous measurement of several orders of reflection at fixed geometry of the experimental arrangement (Michalec and Mikula, IV. Intern. School on Neutron Physics, Dubna, 1982).

1. Double crystal rocking curves of perfect Si single crystals were studied. The departure of the observed rocking curve form from the dynamical one increasing with the order of reflection is explained in terms of vertical beam divergence and vertical misorientation angle $\emptyset_0$. Fig.1 displays the results obtained for the 440 reflection.

2. The study of neutron back-scattering on a bent Si crystal proved that the integrated reflectivity is enhanced only by the variation of the interplanar distance d_{hkl}. At higher orders of reflection a considerable gain in intensity (fig.2) can be achieved in this way without major losses in energy resolution.

3. Thermal diffuse scattering of neutrons on a thick perfect Si crystal affects most distinctly the intensity of higher order reflections (fig.3).

A new facility DIFRAN is under construction being intended for a wide spectrum of experiments in the study and application of dynamical neutron diffraction at the IBR-2 pulsed reactor at JINR, Dubna (Alexandrov et al., VII. Conference of Czech. Physicists, Prague,1981).

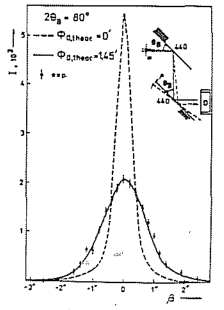

Fig.1.

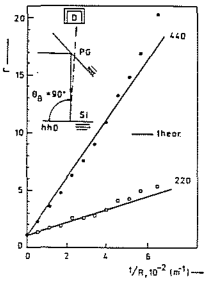

Fig. 2.

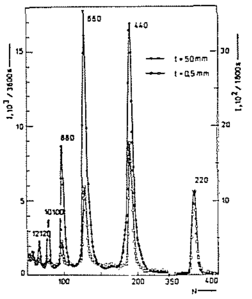

Fig. 3.

11.7–29 CREATION OF NEW WAVEFIELDS IN DISTORTED CRYSTALS.

By J. Gronkowski, University of Experimental Physics, Varsaw, Poland and C. Malgrange, Laboratoire de Minéralogie-Cristallographie, Université Pierre et Marie Curie, Paris, France.

Although well evidenced phenomenologically for quite a long time, the creation of new wavefields (interbranch scattering) in highly distorted crystals was accounted for analytically only quite recently (F. Balibar, F. Chukhovskii, C. Malgrange, Acta Cryst. (1983) A39,387) for a constant strain gradient using an expansion of the Green function in the reciprocal space. The most important results of that theoretical approach were :

1. a demonstration that a new wavefield is created only if the tie-point of the original wavefield passes through the apex of the dispersion surface.
2. a simple analytical formula for the intensity of the phenomenon.

Allowing a conjecture included in that paper, the present authors performed a computer experiment with Takagi's equations and were able to show that these results were readily extendable to variable strain gradients (J. Gronkowski, C. Malgrange (1984) submitted to Acta Cryst.). The intensity of the newly created wavefield was shown to depend only on the value of the strain-gradient in the immediate vicinity of the region where the creation takes place. Even for highly distorted crystals, the basic equations of geometrical optics were shown to be valid if one considers separately the original wavefield and the new one. The applicability of such a combined approach (geometrical optics and analytical formula for the creation of new wavefields) to practical cases, e.g. the contrast of dislocations, will also be highlighted.