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Neutron diffraction by an absorbing vibrating InSb crystal.

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Abstract

Following our recent paper [Lukáš, Kulda, Mikula, Sedláková, Alexandrov & Vrána (1991). *Acta Cryst.* A47, 166-169], a comparison of the dynamical description of diffraction by an absorbing elastically deformed perfect crystal with the experimental data taken at diffraction by a longitudinally vibrating InSb crystal is presented. The comparison is performed on the time-dependent integrated intensity spectra for different values of the vibration amplitudes. The applicability of the analytical formulas derived earlier by two of the authors for an arbitrary homogeneous deformation is in this case fully approved by the good agreement between the theory and the experiment.

In a recent paper (Lukáš *et al.*, 1991) we have presented the results of neutron diffraction studies on the reflectivity of Si and absorbing InSb perfect crystals elastically deformed by a temperature gradient. The experimental data collected at several reflection orders were treated in terms of theoretical formulas derived earlier in a set of papers by Kulda (1984), Lukáš & Kulda (1987) and Kulda & Lukáš (1989). Now we continue the tests of these reflectivity formulas for another kind of deformation featuring a time-dependent strain gradient. The present experiments were carried out on the TKSN-400 diffractometer in Řež with a highly perfect absorbing InSb crystal excited into longitudinal vibrations, which is considered below as a pure one-dimensional deformation. Reflectivity properties of pure one-dimensionally deformed nonabsorbing crystals were shown earlier in papers by Guigay (1986) and Guigay, Mikula, Hock, Baruchel & Waintal (1990).

Diffraction was performed on the (220) lattice planes of an InSb crystal with dimensions $50\times10\times8$ mm and set in symmetric transmission geometry. Longitudinal vibrations at the resonance frequency of 10 kHz were excited by piezoceramics stuck to the middle of the crystal bar (see Fig. 1). An incident beam (width 10 mm) of neutrons with wavelength $\lambda = 1{\cdot}02$ Å was monochromatized by a Zn(002) mosaic crystal and entered the crystal bar near to one end (Fig. 1). The diffracted beam was detected by a thin ^{6}Li glass scintillator connected to a multichannel analyser with a T/D convertor having a channel width of 3 μs. In this experimental arrangement we observed the time-dependent integrated intensity spectra for different vibration amplitudes which are displayed in Fig. 2.

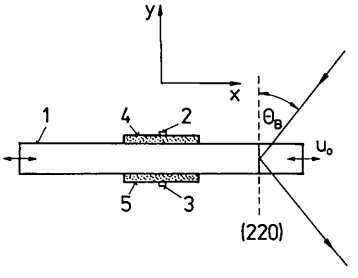

Fig. 1. Schematic diagram of diffraction by a longitudinally vibrating crystal bar: 1, crystal; 2, 3, holding points; 4, 5, exciting and controlling piezoceramic plates.

The intensity against channel number dependence was fitted by the following model:

$$I_j = A_1\rho_Y[\Delta Y_j(n)] + A_2, \qquad (1)$$

where the intensity scale factor A_1 and an additive contribution A_2 arising from the background and thermal diffuse scattering are free parameters, n is the channel number proportional to the time. In the course of the fit common values of the parameters A_1 and A_2 were employed for all measured spectra which were taken for different vibration amplitudes and individually numbered by the index j. The formula for integrated reflectivity $\rho_Y(\Delta Y)$ as well as for the dimensionless parameter ΔY can be found in the paper by Lukáš *et al.* (1991). ΔY describes the total variation in Bragg angle for the incident beam along its path through the crystal.

The angular deviation $\theta - \theta_B$ brought about by moving the lattice planes of the longitudinally vibrating bar and dependent on the coordinate x (see Fig. 1) and the time t is given by (Kulda, Vrána & Mikula, 1988)

$$\theta - \theta_B = \Delta\theta_s - \frac{u_0\pi}{L\cos\theta_B}[\sin\theta_B\cos(\pi x/L)\sin\omega t + (c_x/v_n)\sin(\pi x/L)\cos\omega t], \qquad (2)$$

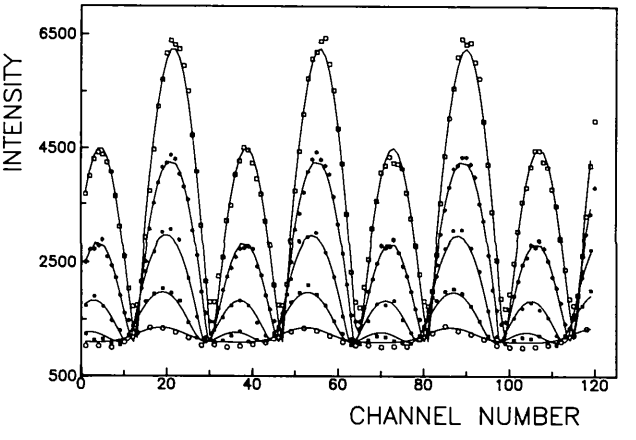

Fig. 2. Time-modulated integrated intensity of the longitudinally vibrating perfect-crystal bar of InSb for different values of the dimensionless deformation-gradient amplitude ΔY_j^{max} being equal to 1·0 (○), 3·6 (■), 8·1 (●), 14·7 (*) and 25·1 (□), respectively.

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where θ_B, u_0, L, ω, v_n and c_x are the Bragg angle, the vibration amplitude, the length of the crystal, the angular frequency, the neutron velocity and the velocity of propagation of ultrasonic waves in the crystal, respectively. The constant parameter $\Delta\theta_s$ means the angular deviation at the point where the neutron enters the crystal and is determined by setting the crystal with respect to the incident-beam direction. The time-dependent total change in Bragg angle $\Delta Y_j(n)$ was fitted in the simplified form

$$\Delta Y_j(n) = A_j \sin(A_{j+1}n + A_{j+2}), \quad (3)$$

where

$$A_j = \frac{2\pi^3 \Omega u D \tan\theta_B}{\lambda^2 L^2 F_G}\left(\frac{c_x^2}{v_n^2} - \sin^2\theta_B\right)$$

contains the vibration amplitude u and known constants such as the structure factor F_G, the crystal thickness D *etc.* A_{j+1} and A_{j+2} correspond to the circular frequency and the phase factor, respectively. It should be pointed out that the time $\Delta t = D/(v_n \cos\theta_B)$ which a neutron spends in the crystal is much smaller than the vibration period and consequently the crystal deformation which the neutron meets on its path may be considered homogeneous to a good approximation.

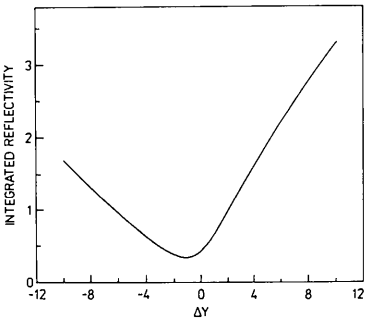

Fig. 3. Theoretical dependence of the integrated reflectivity of an InSb(220) crystal as a function of ΔY for the neutron wavelength $\lambda = 1{\cdot}02$ Å.

Inspection of Fig. 2 shows a good agreement between the theory and the experimental results. For a better understanding of the results obtained we show the theoretical dependence of the integrated reflectivity on a static deformation ΔY (Fig. 3). Depending on the deformation-gradient direction with respect to the scattering vector, one of the two different wavefields is excited in the crystal. The attenuation coefficients of these wavefields differ from each other and therefore the reflectivity is not symmetric on the ΔY scale with respect to zero (see Fig. 3). In the vibrating crystal, these individual wavefields are excited in each half-period of vibration and for this reason different heights of neighbouring maxima are observed in the spectra displayed in Fig. 2.

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Strukturverfeinerung des Kompositkristalls im mehrdimensionalen Raum: Identifizierung der verschiedenartig aufgestellten Superraumgruppen.

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Abstract

Different settings of the superspace group of a composite crystal often appear as if they were different superspace groups. To identify them, a method has been developed which includes a transformation of the superspace unit cell into a reduced one and a provisional definition of the reduced cell in higher dimension has been proposed.

Einleitung

Um die unbekannte Struktur eines Kompositkristalls zu bestimmen, löst man zunächst die mittleren Strukturen der Teilsysteme in voneinander getrennten Verfahren. Die Teilstrukturen werden dann in einen mehrdimensionalen Raum eingebettet, um unter einer Superraumgruppe verfeinert zu werden (Janner & Janssen, 1980; Kato, 1990). Die mögliche Superraumgruppe läßt sich aus den Raumgruppen der Teilstrukturen ableiten (Kato & Onoda, 1991*b*). Hierbei wird die erstere je nach den Aufstellungen der letzteren und/oder nach der Wahl des Minimalsystems verschiedenartig aufgestellt. Bei mehreren, scheinbar verschiedenen Angaben der Superraumgruppen für einen Kompositkristall muß man daher feststellen, ob es sich bloß um verschiedene Aufstellungen der gleichen Superraumgruppe oder aber tatsächlich um verschiedene Superraumgruppen handelt. Hierzu wäre es angebracht, zunächst die mehrdimensionale Elementarzelle in eine reduzierte Zelle zu transformieren und dann die Symmetrieoperationen in ihrer entsprechend

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