angles the effect on the thermal parameters may be appreciable.

On some occasions the polarization ratio $K$ has been included in the parameters that are refined. The results have not been encouraging as the values may have fallen far outside the bounds of direct determinations (Vincent & Flack, 1980; Bachmann, Kohler, Schulz & Weber, 1984). This is not very surprising in the light of the above findings, which demonstrate that a smooth angular function can be absorbed in the model in many different ways.

The users of diffractometers are urged to determine $K$ experimentally, or at least to make an estimate as outlined in the Introduction. The values given in Table 1 suggest that the dynamical value for $K$ is a better estimate than the customarily used kinematical value. Jennings (1984) lists 40 determinations of $K$ in a survey conducted for the International Union of Crystallography Commission on Crystallographic Apparatus. These results also give guidelines for an estimation of $K$.

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References


Neutron Diffraction from Single-Crystal Silicon: the Dependence of the Thermal Diffuse Scattering on the Velocity of Sound

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Abstract

It is well known [Willis (1970). Acta Cryst. A26, 396-401] from the theory of one-phonon scattering of thermal neutrons by a crystal that the nature of the thermal diffuse scattering (TDS) near the Bragg peak depends on whether the neutron velocity is greater than or is less than the sound velocity in the crystal. For faster-than-sound neutrons the TDS rises to a peak coinciding with the Bragg peak, whereas for slower-than-sound neutrons the TDS tends to give a flat background across the Bragg reflection. These theoretical predictions are supported by experiments using pulsed neutron diffraction from single crystals of perfect silicon. In particular, the integrated TDS across a reflection undergoes a pronounced fall when the neutron velocity drops below the velocity of sound.

1. Introduction

In a diffraction experiment, with either a single crystal or a polycrystalline sample, the measured intensity of a Bragg reflection will include a contribution from thermal diffuse scattering (TDS) which arises from the scattering of the incident beam by phonons. For X-rays, the one-phonon TDS is not subtracted with the background measured on either side of the reflection, since it rises to a maximum at the same point as the Bragg peak itself. This then causes the so-called TDS error in estimating Bragg intensities.

For thermal neutrons, the situation is quite different (Willis, 1970). The reason is that the neutron energy is comparable with the phonon energy, whereas X-rays have energies that are five orders of magnitude higher. Consequently, the condition

$$|\mathbf{k}| = |\mathbf{k}_0|$$

(1)

(where $\mathbf{k}$ and $\mathbf{k}_0$ are the wave vectors of the scattered

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and incident radiation respectively) for the one-phonon scattering of X-rays does not apply to neutrons. Instead we must write

$$|k| = |k_0| - \varepsilon \beta q,$$

(2)

where the extra term, $\varepsilon \beta q$, is comparable in magnitude with $|k| - |k_0|$. $\varepsilon$ in (2) is either $+1$ or $-1$: $\varepsilon = +1$ corresponds to phonon emission (creation) and $\varepsilon = -1$ to phonon absorption (annihilation). $\beta$ is the ratio of the velocity of sound in the crystal to the neutron velocity, and $q$ is the wave number of the phonon associated with the scattering process. It is assumed in (2) that $q < k_0$ (i.e. that the TDS is close to the Bragg position) and that the velocity of sound associated with each acoustic mode is isotropic.

Before calculating the intensity of the TDS at a given setting of the crystal it is necessary to define the locus in reciprocal space of the end point of the phonon wave vector $q$. This locus is referred to as the scattering surface. [The phonon wave vector $q$ joins the end points of the scattering vector $(k - k_0)$ and the reciprocal-lattice vector.] For X-rays this locus coincides with the Ewald sphere in accordance with (1), but for neutrons it is more complicated. From (2) the end point of $q$ lies on a conic of eccentricity $1/\beta$.* If the neutrons are faster than sound ($\beta < 1$), the locus is a hyperboloid of two sheets, with the $q$ vectors on one sheet corresponding to emission of phonons and on the other sheet to absorption. If the neutrons are slower than sound ($\beta > 1$), the locus is an ellipsoid: scattering now occurs either by emission or by absorption but not by both together.

These two types of neutron scattering surface are illustrated in Fig. 1.

* This is strictly correct for $\theta = 0$ only. For $\theta > 0$, the eccentricity is $1/(\beta \cos \theta)$: see § 3 for the origin of this geometrical term.

Knowing the geometry of the scattering surface for each setting of the crystal, and applying standard formulae for the one-phonon scattering cross section associated with each $q$ vector lying on the surface, we can calculate easily the integrated TDS intensity, $I_{\text{TDS}}$, lying above the straight-line background across the Bragg peak. The results are (Cooper, 1971):

(a) X-rays. The TDS rises to a maximum at the Bragg peak and the TDS error can be derived if the elastic constants of the crystal are known.

(b) Neutrons: $\beta < 1$. The TDS rises to a maximum, just as for X-rays, and $I_{\text{TDS}}$ is obtained using the same formulae as for X-rays with the scattering factor for X-rays replaced by the neutron scattering amplitude. [This is a remarkable result in view of the different scattering surfaces for (a) and (b).]

(c) Neutrons: $\beta > 1$. The variation in intensity of the TDS is much less pronounced than for (a) and (b). For a given value of $q$, the integrated intensity per mode is proportional to $1/q^2$. However, the number of modes participating in the scattering falls as the scattering surface approaches the reciprocal-lattice point, and the two effects combine to produce a flat TDS background near the Bragg peak. $I_{\text{TDS}}$ is then zero.

In this paper we shall describe an experiment on silicon illustrating the sharp distinction between cases (b) and (c). The neutron Laue technique was used as this is a convenient method of determining $I_{\text{TDS}}$ as a function of neutron wavelength.

2. Experiment

The single-crystal Laue method with neutrons was first proposed by Buras & Leciejewicz (1964). Polychromatic neutrons are scattered at a fixed angle $2\theta$ by the sample and the time-of-flight technique is used to separate the detected neutrons in accordance with their wavelength. The time of flight, $t$, for neutrons of wavelength $\lambda$ is related to the total length of the flight path, $L$, by

$$\lambda = 0.003955 t / L,$$

(3)

where $\lambda$ is in Å, $t$ in μs and $L$ in m. The timing measurement requires the initial production of neutron pulses, no more than a few μs in duration, which disperse themselves in time as they travel to the sample and are then scattered to the detector.

The neutron source for the present experiment was the Harwell electron linear accelerator Helios (Lynn, 1980) which was operated at a pulse repetition frequency of 75 Hz – sufficiently small to avoid frame overlap between successive pulses. A single crystal of dislocation-free silicon, in the form of a circular disc 50 mm in diameter and a few mm in thickness, was mounted on large goniometer arcs and placed on the $\omega$-rotation table of the diffractometer which has a flight path, $L$, from the moderator to the detector.
of 11.96 m. The arcs had been adjusted previously to bring the [220] axis, lying in the plane of the disc, into the horizontal plane. The [112] axis of the crystal was normal to this plane. The detector was set at a fixed angle $2\theta$ in the range 20° to 60°, the [220] axis set at $90° - \theta$ to the incident beam, and intensity measurements carried out of the $hh0$ zone of reflections (see Fig. 2). The widths of the time channels chosen for the multi-channel analyser were 2 or 4 $\mu$s and the total time of counting at a given $2\theta$ was four days.

Fig. 3 shows some typical data, illustrating the Bragg and thermal diffuse scattering associated with the 220 and 440 peaks. The TDS is particularly pronounced since its intensity is governed by the kinematic conditions of scattering, whereas the Bragg intensity for a perfect crystal is limited by dynamical diffraction and is independent of the thickness $t$ of the crystal (apart from weak Pendellösung oscillations) for $t$ exceeding the extinction distance. The background in Fig. 3 is flat at a sufficiently large distance from the peaks and is extrapolated as a broken line under the peaks.

The integrated intensity (Bragg+TDS) was measured above this broken line, and $I_{\text{TDS}}$ was separated from the integrated Bragg intensity by estimating the latter from the longest-wavelength diffraction peaks where the TDS is known to be flat. The total integrated intensities for the $hh0$ reflections were measured at four different scattering angles. These results are analysed in the next section.

3. Analysis of experimental data

Firstly, we assume that the TDS under the Bragg peak arises entirely from one-phonon scattering. (Multi-phonon scattering will be largely subtracted in the background measurement.) Using the kinematic theory for the one-phonon scattering of neutrons of fixed wavelength $\lambda$, and making the somewhat drastic assumption that the volume scanned is a sphere centred on the reciprocal-lattice point, we find that the integrated intensity of one-phonon scattering $I_{\text{TDS}}$...
The Intensity Fringes of Three Coupled Waves in Crystals

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Abstract

Two different kinds of interaction between three waves $D_0$, $D_h$ and $D_e$ in a perfect crystal are investigated in the case of Laue scattering using the Takagi-Taupin equations. Polarization effects (coupling between $\sigma$ and $\pi$ waves) are neglected, and it is assumed that the incoming vacuum wave $D_0^{(\sigma)}$ has a small wave-front area whose spatial extension is simulated by a point source on the crystal surface. The solutions of the diffraction equations thus constitute the boundary-value Green functions for the wave

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