It is also restricted to the case that each type of stacking fault 'produces' only one new type of unit cell in the material.

The intensity distribution of a powder diagram line is described by equation (26) with the same limitations as for equation (25). The quantities $\varphi(t; L)$ and $C(t)$ in equation (26) can be replaced by $\varphi''(t; L)$ and $C''(t)$, chosen such that $\varphi''(t; L)=0$ for $L \geq \frac{1}{2}d$. This provides also a right description of the intensity distribution of a Debye–Scherrer line. The quantities $\varphi''(t; L)$ and $C''(t)$ can be found from the line profiles; the corresponding unprimed quantities cannot be found from a powder diagram, unless a model of the distortions is assumed.

The intensity distributions given in equations (25) and (26) are still unnormalized. When one wishes to determine the distribution of the distortions and the form function of the average coherently scattering region it is necessary to know the normalization constant to within the factor N. To find that constant, equation (26) is integrated over s_0

$$\begin{aligned}
&\int_{-\infty}^{+\infty} I_l(s_0)\mathrm{d}s_0 \\
&\quad = \int_{-\infty}^{+\infty} \mathrm{d}s_0 \sum_{pp'} f_p f_{p'}^* \int_{-\infty}^{+\infty} C(t) G_{pp'}(t; s_l) N_{pp'}(t) \\
&\quad \times \exp(2\pi i s_0 t) \int_{-\infty}^{+\infty} \varphi(t; L) \exp(2\pi i s_l L)\mathrm{d}L \\
&\quad = \sum_{pp'} f_p f_{p'}^* \int_{-\infty}^{+\infty} \delta(t) G_{pp'}(t) N_{pp'}(t)\mathrm{d}t \\
&\quad \times \int_{-\infty}^{+\infty} \varphi(t; L) \exp(2\pi i s_l L)\mathrm{d}L \\
&\quad = N_{oo}(0) f_o f_o^* + N_{11}(0) \sum_{p\neq o} 2\mathrm{Re} f_o f_p^* . \qquad (52)
\end{aligned}$$

Here we used $G_{pp'}(0)=1$ and $N_{pp'}(0)=0$ if $p, p' \neq 0$. Equation (52) holds when all glide plane directions are equivalent by the symmetry of the structure, or, when $N_{op}(t)=0$ for $p\neq 0$ and $p\neq 1$. We have for these cases:

$$kN_{11}(0) = N - N_{oo}(0) . \qquad (53)$$

Where k is the number of types of stacking faults. Thus the inverse of the normalization constant is:

$$\int_{-\infty}^{+\infty} I_l(s_0)\mathrm{d}s_0 = f_o f_o^* N_{oo}(0) + \frac{N - N_{oo}(0)}{k} \sum_{p\neq o} \{2\mathrm{Re} f_o f_p^*\} . \qquad (54)$$

Once the stacking-fault density κ is known, one can calculate the normalization constant to within the factor N by means of relations (53) and (54) and the relation

$$\kappa = N^{-1} N_{11}(0) . \qquad (55)$$

A final remark should be made. In equations (44), (49), (50) and (51) we disregarded the special case, that one of the glide plane directions is perpendicular to $\mathbf{s}_n$. Then, for that type of stacking-fault, $N^{-1}N_{op}(t)$ equals zero instead of κ, and that value should be substituted into equations (41) and (42). Of course κ can be substituted for all other types of stacking faults. The equations (49), (50) and (51) can be adapted immediately by omitting F_p^{im} and F_p^{re} for that type of stacking fault.

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Crystal Measurements for Absorption Correction

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A method is described for determining, with few measurements and calculations, the bounding planes of a crystal.

The availability of computer programs for absorption correction by either the Gaussian integration or analytical methods (Ahmed, 1970) means that these corrections can be calculated for polyhedral crystals to any desired accuracy. This suggests that it may be preferable not to grind crystals into spheres, a proce-

dure that often cannot be applied, and that frequently produces ellipsoids rather than spheres, introducing a further error that is very difficult to remove.

The problem then becomes simply one of measuring and describing the crystal as exactly as possible, and this note presents a simple method of doing so. A perfect crystal can be described equally well by its vertices or faces, but if it is slightly damaged or irregular, the faces are likely to be more easily identified and located. This can be done goniometrically, and indices assigned to each face, but this may require rather complex calculation; also with an irregular crystal, the 'best' bounding surface may not be a crystallographic plane. By the present method, the equations of the bounding faces are directly determined with a minimum of measurement and calculation. They are referred to orthogonal axes, which can be used directly in some absorption programs if the crystal is suitably oriented (Alcock, 1969) or can be converted to any other axis set.

A generally similar method has been developed by H. A. Levy and is described by Busing (1969), which is probably more accurate if the bounding planes are crystallographic planes, but involves the use of a four-circle diffractometer with a telescope mounted independently of the χ and φ circles.

Theory

If the crystal is rotated, while being viewed perpendicular to the axis of rotation through a microscope or telescope, then every face will, at some position, be 'eclipsed' so that it is parallel to the line of view (excepting basal and apical planes which are always eclipsed).

Fig. 1 shows a crystal in which two planes are in this configuration. Taking the axis of rotation as the z axis, Fig. 2 shows the traces of these planes in the $x-y$ plane. If the normal to the trace of one plane is D_1 and its polar coordinate φ_1, then its equation is

$$x\cos\varphi_1+y\cos(\varphi_1-90)=D_1 \qquad (1)$$

and the equation of the crystal plane must be

$$x\cos\varphi_1+y\cos(\varphi_1-90)+Kz=D_1\,. \qquad (2)$$

If the acute angle between the eclipsed plane and the z axis is θ_1 (Fig. 1) then the plane cuts the z axis at

$$z=\pm D_1/\tan\theta_1 \qquad (3)$$

i.e. K in equation (2) is $\pm\tan\theta_1$. The + or − sign depends on whether the intersection is towards + or $-z$. Thus the plane is defined by means of the three quantities, D, φ and θ.

Typical procedure

The crystal (on a goniometer head) is positioned under the microscope so that it can be rotated through a measurable angle, perpendicular to the microscope axis (assumed vertical) and also rotated with the microscope stage, and translated to bring the crystal into view. A suitable device is the Nonius crystal orienter (adapted to attach to the stage) on which a dial indicates the angle of rotation of the crystal. The microscope eyepiece is equipped with some means of measuring distance fairly precisely (*e.g.* a Vickers screw micrometer eyepiece, which incorporates a slide wire moved by a calibrated drum).

The dial reading (ψ_0) at which the x axis is pointing up is determined or defined. [This could be when a^* is vertical if the crystal is mounted about c (Alcock, 1969)]. The crystal is moved by the goniometer head slides until the rotation axis, which will be the z axis, passes through it. The eyepiece (or stage) is rotated until this axis is perpendicular to the measurement direction, and the crystal is moved until the line on which measurements will be taken (to be the $x-y$ plane) intersects as many faces as possible.

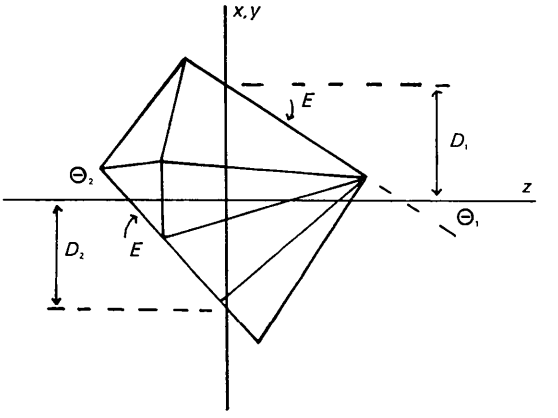

Fig. 1. View of a crystal rotated until two planes (marked E) are eclipsed. The x and y axes are in the plane marked x,y.

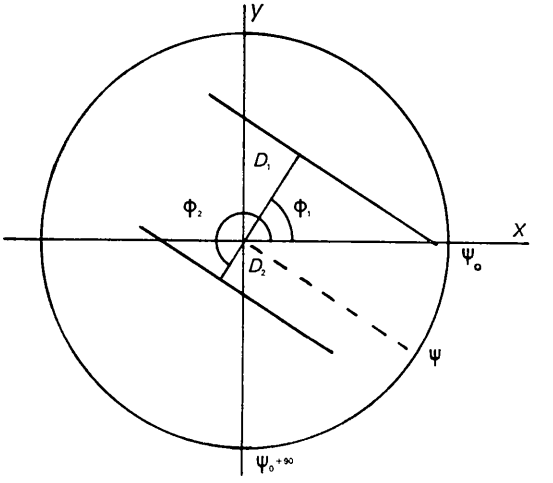

Fig. 2. View of the $x-y$ plane ($+z$ out of the paper), with traces of two crystal planes. The polar coordinates (φ) and the dial angles (ψ) are also shown.

Then the crystal is rotated until each face is eclipsed. The dial angle (ψ_A) and the scale reading (D_A) where the face cuts the x, y line are noted; the crystal is then rotated through 180° and the measurements repeated (ψ_B, D_B). To obtain θ, the stage is rotated until each face, in its eclipsed position, is parallel to one of the crosswires. A note is also made of whether the face interesects the $+z$ or $-z$ axis. If the relationship between ψ and the $x-y$ direction is as in Fig. 2 then $\varphi=90-(\psi-\psi_0)$, where ψ is the dial reading when the plane is on the 'positive' side of the z axis (*i.e.* the side to which $+y$ projects when the x axis is vertical). The distance D, from the z axis is given by half the difference between D_A and D_B, while the z axis cuts the $x-y$ plane at a scale value D_A+D. The plane equation is then:

$$x \sin(\psi-\psi_0)+y \cos(\psi-\psi_0)\pm z \tan\theta=\tfrac{1}{2}(D_B-D_A)\,.$$

For example:

$\psi_0=256°$. 1 drum unit=0·00004283 cm. Positive side of z axis is to the lower scale value.

$\psi_A=64°$, $D_A=376$ drum units.

$\psi_B=244°$ $D_B=596$ drum units.

$\theta=20°$ intersecting $+z$ (away from the goniometer head).

This gives $D=110$, the z axis is at 486, $\psi=\psi_A-\psi_0=168°$, and the plane is:

$$x \sin 168+y \cos 168+z \tan 20=110*0{\cdot}00004283$$

or

$$0{\cdot}2079\,x-0{\cdot}9871\,y+0{\cdot}3640\,z=0{\cdot}004711\,.$$

For planes which do not cut the $x-y$ line, two courses are possible. If, when eclipsed, they cut the crosswire parallel to the z axis (at 500 units on the screw-micrometer eyepiece) the eyepiece can be rotated through 90° and the distance of this intersection from the $x-y$ line measured. Then, using θ, the intersection of the eclipsed plane with the z axis can be calculated (D_z) and then the distance $D=D_z \cos\theta$. For a basal plane, of course, the equation is simply:

$$z=D_z\,.$$

Alternatively, the distance (parallel to the z axis) to some prominent point can be measured (by rotating the eyepiece), the crystal translated until this point lies on the $x-y$ line, and a further series of measurements made with a new origin, and referred to the first origin.

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Artificial Splitting of One-Phonon Neutron Groups due to Relaxed Vertical Collimation

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It is shown that in certain circumstances the relaxed vertical collimation of a triple-axis spectrometer can lead to the measured one-phonon neutron groups having two peaks, and experimental measurements which clearly show the splitting and indicate its origin are presented. In the form of dispersion curve considered, two branches of the curves are degenerate along a symmetry direction but split for any adjacent wave vector with the splitting directly proportional to the distance from the symmetry direction. An additional requirement is that the resolution function of the spectrometer should be squashed along the symmetry direction and expanded perpendicular to it. Calculations which also show the splitting of the neutron groups are described.

Introduction

In inelastic neutron scattering experiments performed with a triple-axis spectrometer, it is customary for the vertical divergence of the spectrometer to be greater than the horizontal divergence by a factor of two or three. Whenever possible specimens are mounted with a mirror plane horizontal. This normally results in the frequencies of the observed phonons or magnons not changing, to first order, for wave vectors slightly out of the scattering plane. The relaxed vertical collimation then leads to a useful increase in intensity with negligible broadening of the neutron groups. The presence of a mirror plane is not, however, sufficient to ensure that the constant frequency surfaces cut the scattering plane normally. If two branches of the dispersion curve are degenerate along a line in the scattering plane, for wave-vectors with a small off-symmetry-