time-dependent molecular trajectories calculated in a molecular dynamics study (Dove, Fincham & Hubbard, 1986); a detailed study of the diffuse scattering from a single crystal of SF_6 is still missing.

The occurrence of the maxima of diffuse intensity in C_2Cl_6 at wavevectors slightly larger than the (111) planes in reciprocal space might be a hint to a rotational-translational coupling connected with the orientational ordering: the attractive forces between two parallel orientated nearest-neighbour molecules cause a decrease in the centre-of-mass distance of about 8%.

A remarkable experimental fact is the complete absence of well defined collective translational excitations. While it is well known that librational modes are usually overdamped in ODIC phases of molecular crystals, it is surprising that no acoustic modes could be resolved, even at small wavevector transfers. It is difficult experimentally to extend the investigation closer to the Brillouin-zone centre, because elastic scattering from misaligned crystallites leads to spurious peaks in this region. The analysis of the energy-integrated scattering has shown that the thermal diffuse scattering due to phonons is relatively weak in comparison with the orientational disorder scattering. This suggests that the translational displacements are also of overdamped character probably due to a strong translational-rotational coupling. SF_6 is another example where a similar measurement (Dove, Pawley, Dolling & Powell, 1986) revealed no well defined acoustic modes, in contrast to most other orientationally disordered crystals (*e.g.* CD_4, CBr_4, N_2) in which the acoustic phonons are well defined, at least at small wavevectors.

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A General Lorentz Correction for Single-Crystal Diffractometers

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Abstract

A single-crystal Lorentz correction is derived for the case of a general scan through an out-of-plane reflection on a four-circle diffractometer with relaxed sample-to-detector collimation. When the Lorentz correction is expressed in terms of the incremental steps in the Eulerian setting angles, structure amplitudes observed by different scan trajectories, for example, some angular in real space and others linear in reciprocal space, are put on a common scale, and errors due to known missetting of the angles or rounding off of the angles are avoided.

Introduction

In a conventional single-crystal diffraction experiment the integrated intensities of the reflections are measured by rotation of the crystal about one axis of the diffractometer, usually that axis which best resolves neighbouring reflections. For a constant velocity of rotation of the crystal, different reciprocal-lattice points pass through the Ewald sphere at different rates and therefore have different times-of-reflection opportunity. The inverse of the correction factor to be applied to the observed integrated intensities to obtain (relative) squared structure amplitudes is called the Lorentz factor, following the demonstration of its dependence on the experimental arrangement by Lorentz in one of his classroom lectures (Azaroff, 1968).

For some structures, particularly those which are incommensurate or exhibit macroscopic stacking

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faults along one axis, it might be preferable to perform linear scans in reciprocal space rather than pure rotational scans in real space, or to combine data sets obtained by both types of scans. Note that linear refers to the trajectory of the *detector aperture* through reciprocal space. For a *particular reflection* observed in this scan, the motion of the corresponding reciprocal-lattice point through the Ewald sphere is still along an angular trajectory (Fig. 1). Lebech & Nielsen (1975) have derived the Lorentz factor for linear reciprocal-lattice scans for the case of a two-axis equatorial-plane diffractometer.

While it is usually desirable to restrict the scans to the equatorial plane in order to take best advantage of the resolution of the diffractometer, in general, scans might be performed at an angle to the equatorial plane through reflections that do not lie in the equatorial plane. In this paper we derive and discuss the application of a general Lorentz correction that is valid for any scan through a general out-of-plane reflection. Axe & Hastings (1983) presented general expressions for the Lorentz factor for samples with arbitrary horizontal and vertical mosaic on two- and three-axis spectrometers. In the present derivation, however, we assume that the sample mosaic is negligibly small, and that the sample-to-detector collimation is relaxed so that the detector receives all the scattered radiation from the reflection under consideration.

Angle definitions

To derive the Lorentz factor for specific scan geometries we adopt the definitions of Busing & Levy (1967) for the Eulerian angles χ and φ defining the crystal orientation. We denote however their ν by ω, since our definition corresponds to the physical angle ω on most modern four-circle diffractometers. We also adopt their definitions for the frames of reference attached to the crystal, the orienter axes and the laboratory, and their nomenclature for the matrices **B**, **U**, **Φ**, **X**, and **Ω** that transform a vector from one frame to another (except that their matrix **N** corresponds to our matrix **Ω**). In addition, to allow for out-of-plane reflections, as might be scanned on a normal-beam diffractometer or on a four-circle diffractometer equipped with a large-area position-sensitive detector (PSD), two angles are required to specify the direction of the diffracted beam. These are γ, the angle made by the projection of the diffracted beam onto the equatorial plane with the incident beam, and ν, the angle of the diffracted beam out of the equatorial plane (Fig. 1). 2θ remains the angle between the incident and diffracted beams.

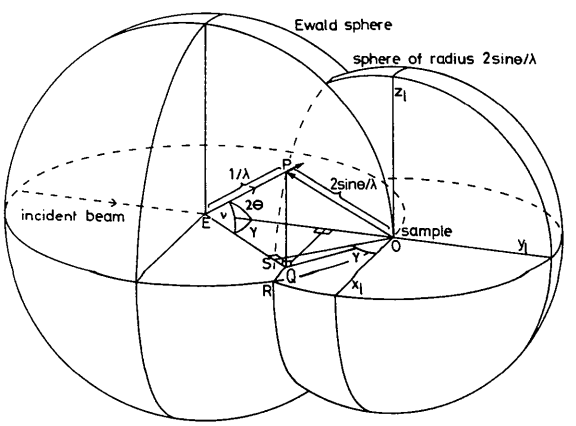

Fig. 1. Ewald construction for an out-of-plane reflection. E is the centre of the Ewald sphere, O is the sample position and origin of the reciprocal lattice and P is the tip of the scattering vector **k** of length $2(\sin\theta)/\lambda$. The diffracted beam and the scattering vector are along EP and OP respectively. Whatever the trajectory of the scan the tip of the scattering vector moves over the surface of the sphere with radius $2(\sin\theta)/\lambda$.

The integrated intensity

The square of the structure-factor amplitude, $|F_{hkl}|^2$, is proportional to the background-corrected intensity per unit time of the reflection *hkl* integrated over reciprocal space. If the (continuous) function $I(x, y, z)$ is the background-corrected intensity distribution in reciprocal space in the vicinity of the reciprocal-lattice point *hkl*, then,

$$|F_{hkl}|^2 \propto \int I(x, y, z)\, dx\, dy\, dz,$$

where x, y, z are the axes of an arbitrary Cartesian coordinate system in reciprocal space. For a particular reflection we can define x, y, z to be the local Cartesian coordinate system with origin at the point *hkl* such that the unit vectors **x** and **y** defining the x and y axes lie tangent to the Ewald sphere, and the unit vector **z** defining the z axis is perpendicular to the Ewald sphere. **z** is also along the diffracted beam. The integration over x and y, for each section z, corresponds to $I_{xy}(z)$, the background-corrected total count observed at the point z in the scan. Thence,

$$|F_{hkl}|^2 \propto \int I_{xy}(z)\, dz.$$

For a single detector, $I_{xy}(z)$ is the background-corrected count received through the detector aperture at the point z; for a PSD, $I_{xy}(z)$ is the background-corrected sum of the counts over an area on the PSD in the vicinity of the reciprocal-lattice point.

In general, however, the direction of motion of the reciprocal-lattice point through the Ewald sphere is not parallel to **z**. Instead, I_{xy} is measured as a function of some scan variable s, so that,

$$|F_{hkl}|^2 \propto \int I_{xy}(s)(dz/ds)\, ds.$$

The scan variable may be, for example, the rotation angle about a fixed axis, or the displacement along

a reciprocal-lattice line through *hkl*. The derivative dz/ds, whose inverse is proportional to the Lorentz factor L, gives the differential dz in the position of the reciprocal-lattice point along the normal to the Ewald sphere corresponding to a differential ds in the scan variable.

Since the interval in s over which I_{xy} is non-zero is usually small, the factor (dz/ds) is evaluated at the peak maximum and taken outside the integral, to give

$$|F_{hkl}|^2 \propto (dz/ds) \int I_{xy}(s)\, ds.$$

The integral $\int I_{xy}(s)\, ds$ is conventionally called the integrated intensity of the reflection, and clearly depends on the scan type. On modern automatic diffractometers a scan is normally carried out by n successive counts at $n-1$ incremental steps Δs_i and the integration is replaced by a summation. Since the steps may be unequal by choice or by mechanical limitations, it is preferable to use a trapezoidal summation:

$$|F_{hkl}|^2 \propto (dz/ds) \sum_{i=1}^{n-1} \Delta s_i [I_{xy}(s_{i+1}) + I_{xy}(s_i)]/2. \quad (1)$$

The Lorentz factor for a rotational scan in real space

For rotational scans in real space a simple general expression for the Lorentz factor can be derived. If $\mathbf{r}$ is the unit vector along the scan axis and $\mathbf{k}$ is the scattering vector, the vector differential in the position of the reciprocal-lattice point for a left-handed rotation dr is

$$\mathbf{r} \times \mathbf{k}\, dr,$$

and the component along the normal to the Ewald sphere is

$$dz = \mathbf{z}.\mathbf{r} \times \mathbf{k}\, dr.$$

Therefore,

$$dz/dr = \mathbf{z}.\mathbf{r} \times \mathbf{k}.$$

The sign of the result, when evaluated, is immaterial since it depends only on the arbitrarily chosen sense of rotation of the reciprocal-lattice point through the Ewald sphere. The result will also contain a multiplier λ^{-1}, where λ is the wavelength, which arises from the radius of the Ewald sphere and gives dimension to the scattering vector $\mathbf{k}$. The Lorentz factor is conventionally taken to be just the angular dependent factors in $(dz/dr)^{-1}$, *i.e.*

$$L^{-1} = \lambda |\mathbf{z}.\mathbf{r} \times \mathbf{k}|.$$

Lorentz factors for the common scan geometries are reported by Lipson (1972) in terms of the angles normally appropriate to these geometries. For later comparison with the generalized Lorentz correction we derive the Lorentz factors for two specific cases.

By inspection of Fig. 1, the vectors $\mathbf{z}$ and $\mathbf{k}$ in the laboratory frame $x_L y_L z_L$ are

$$\mathbf{z} = \begin{pmatrix} \sin\gamma\cos\nu \\ \cos\gamma\cos\nu \\ \sin\nu \end{pmatrix} \quad (2)$$

and

$$\mathbf{k} = (1/\lambda) \begin{pmatrix} \sin\gamma\cos\nu \\ \cos\gamma\cos\nu - 1 \\ \sin\nu \end{pmatrix}. \quad (3)$$

The direction of the scan axis depends on the scan geometry and must be considered separately for each case.

(*a*) *Normal-beam geometry*

The scan axis is the ω axis, $\mathbf{z}_L$, so that

$$\mathbf{r} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

and

$$L^{-1} = \sin\gamma\cos\nu. \quad (4)$$

Equatorial-plane geometry is the special case of normal-beam geometry for which P in Fig. 1 is coincident with R, so that $\gamma = 2\theta$ and $\nu = 0$. Thence,

$$L^{-1} = \sin 2\theta.$$

(*b*) *Flat-cone geometry*

The scan axis is perpendicular to the reciprocal-lattice plane under investigation. For a PSD extended vertically the axis would normally be oriented to lie in the equatorial plane perpendicular to the plane defined by the points E, P and Q in Fig. 1. The scan axis is then along OS, from which follows

$$\mathbf{r} = \begin{pmatrix} \cos\gamma \\ -\sin\gamma \\ 0 \end{pmatrix}$$

and

$$L^{-1} = \cos\gamma\sin\nu.$$

The Lorentz factor for linear scans in reciprocal space

For a step scan along a line in reciprocal space the scan direction could be described by the unit vector $\mathbf{q}$ in a reciprocal-space Cartesian frame [*e.g.* that defined by Busing & Levy (1967)]. The vector differential $\mathbf{q}\, dq$ in reciprocal space is $\mathbf{\Omega X \Phi U q}\, dq$ in the laboratory frame, so that, if the coefficients in the summation of (1) are Δq_i along $\mathbf{q}$, the Lorentz

factor is

$$L^{-1} = \lambda \, dz/dq = \lambda \mathbf{z}.\mathbf{\Omega X \Phi U q}.$$

More commonly though the scan steps are specified as fractional increments Δh_i, Δk_i, Δl_i in all three of the Miller indices h, k, l and Δs_i in (1) is chosen to be just one of these (Δh_i say), even if the scan is inclined to all three axes of the reciprocal unit cell. While this makes specifying the scan commands convenient, it does complicate the calculation of the Lorentz factor since a further factor dq/dh must be included;

$$L^{-1} = \lambda \, dz/dh = \lambda (dz/dq)(dq/dh)$$
$$= \lambda (\mathbf{z}.\mathbf{\Omega X \Phi U q})(\mathbf{q}.\mathbf{B h}),$$

where $\mathbf{h}$ is the reciprocal-lattice vector corresponding to h.

These definitions of the Lorentz factor are consistent with the definition of the Lorentz factor for rotational scans in so far as they correct for the different velocities of the reciprocal-lattice points through the Ewald sphere in the cases of linear scans through different reciprocal-lattice points and linear scans in different directions through the same point. However the different factors are not directly comparable because they do not have the same dimensions; the units of dz/dr are $(\text{Å}^\circ)^{-1}$, while those of dz/dh are $(\text{Å})^{-1}$ and dz/dq is dimensionless. In fact, the magnitude of dz/dh depends on the reciprocal-cell dimensions! Consequently, even though in equatorial-plane geometry a linear scan in reciprocal space along the scattering vector and an $\omega:2\theta$ scan follow the same trajectory with regard to the setting angles ω and 2θ, they do not have the same Lorentz factor.

The number of matrix operations to evaluate dz/dq or dz/dh makes the calculation of the Lorentz factor somewhat tedious. It is computationally more convenient to use the general formulation of $(dz/ds)\Delta s_i$ derived in the next section.

A general Lorentz correction

Rather than evaluate dz/ds for the particular type of scan and then perform the integration over s, we can evaluate $(dz/ds)\Delta s_i$ directly in terms of the incremental steps in the instrumental angles that effect the steps Δs_i. If $\Delta \mathbf{k}_i$ is the vectorial shift in the position of the reciprocal-lattice point corresponding to the scan step Δs_i, the shift along $\mathbf{z}$ is $\mathbf{z}.\Delta \mathbf{k}_i$ which is equivalent to $(dz/ds)\Delta s_i$.

Let the reflection hkl with scattering vector $\mathbf{k}$ diffract at the setting ω, χ and φ. The components of $\mathbf{k}$ in the laboratory frame are given by (3). At the point with setting $\omega + \Delta\omega_i$, $\chi + \Delta\chi_i$, $\varphi + \Delta\varphi_i$ in the general scan through hkl, the scattering vector will have rotated to the position

$$\mathbf{k} + \Delta \mathbf{k}_i = \mathbf{\Omega' X' \Phi' \Phi^{-1} X^{-1} \Omega^{-1} k},$$

where the angular arguments in the transformation matrices $\mathbf{\Omega'}$, $\mathbf{X'}$, $\mathbf{\Phi'}$, $\mathbf{\Phi}^{-1}$, $\mathbf{X}^{-1}$ and $\mathbf{\Omega}^{-1}$ (as defined by Busing & Levy, 1967) are $\omega + \Delta\omega_i$, $\chi + \Delta\chi_i$, $\varphi + \Delta\varphi_i$, $-\varphi$, $-\chi$ and $-\omega$ respectively. Since the ranges in ω, χ and φ over which the reflection is observed are usually small, we can approximate $\cos \Delta\omega_i$ by 1 and $\sin \Delta\omega_i$ by $\Delta\omega_i$ *etc.*, and we can neglect the cross terms of the form $\Delta\omega_i \Delta\chi_i$ *etc.*, to obtain

$$\Delta k = (1/\lambda) \begin{pmatrix} \Delta\omega_i(\cos\gamma\cos\nu - 1) + \Delta\chi_i \cos\omega \sin\nu \\ \quad + \Delta\varphi_i(\cos\chi\cos\gamma\cos\nu \\ \quad - \sin\omega\sin\chi\sin\nu - \cos\chi) \\ -\Delta\omega_i \sin\gamma\cos\nu - \Delta\chi_i \sin\omega\sin\nu \\ \quad - \Delta\varphi_i(\cos\chi\sin\gamma\cos\nu \\ \quad + \cos\omega\sin\chi\sin\nu) \\ -\Delta\chi_i\{\sin(\gamma-\omega)\cos\nu + \sin\omega\} \\ \quad + \Delta\varphi_i\{\cos\omega\sin\chi \\ \quad - \sin\chi\cos(\gamma-\omega)\cos\nu\} \end{pmatrix}. \quad (5)$$

Then, the coefficients of the counts in the summation of (1) are

$$\lambda(dz/ds)\Delta s_i \equiv \lambda \mathbf{z}.\Delta \mathbf{k}_i$$
$$= -[\Delta\omega_i \sin\gamma\cos\nu + \Delta\chi_i \sin\omega\sin\nu$$
$$+ \Delta\varphi_i(\cos\chi\sin\gamma\cos\nu$$
$$- \cos\omega\sin\chi\sin\nu)]. \quad (6)$$

We shall call (6) the general Lorentz correction. According to our derivation the arguments of the trigonometric factors in (6) should be the setting angles at each step through the scan. This is valid only if the wavelength dispersion dominates the resolution function. Removing dz/ds from the integral in (1) is equivalent to evaluating the trigonometric factors at the reflection centre. While this in turn is only valid if the wavelength dispersion and incident-beam divergence are negligible components of the resolution function, it is a sufficient approximation for many diffractometers.

We now consider the form of (6) in some special cases.

(*a*) *Equatorial-plane geometry*

The scattering vector lies in the equatorial plane when it is correctly oriented to diffract ($\gamma = 2\theta$ and $\nu = 0$); the scan however may not necessarily be parallel to the equatorial plane (and $\Delta\omega_i$, $\Delta\chi_i$ and $\Delta\varphi_i$ are in general non-zero);

$$\lambda(dz/ds)\Delta s_i = -[\Delta\omega_i \sin 2\theta + \Delta\varphi_i \cos\chi \sin 2\theta]. \quad (7)$$

This expression applies to *all* scans where the detector remains in the equatorial plane. There is no contribution from $\Delta\chi_i$ since a χ rotation for a reflection in

the equatorial plane moves the scattering vector perpendicular to **z**.

For a pure ω scan (7) reduces to the scan step times the familiar Lorentz factor for an ω scan:

$$\lambda(\mathrm{d}z/\mathrm{d}s)\Delta s_i = -\Delta\omega_i \sin 2\theta.$$

(b) Normal-beam geometry

In the general normal-beam case the crystal may be oriented by all three of ω, χ and φ, but the scan itself is a pure ω scan ($\Delta\chi_i = \Delta\varphi_i = 0$);

$$\lambda(\mathrm{d}z/\mathrm{d}s)\Delta s_i = -\Delta\omega_i \sin\gamma\cos\nu,$$

which agrees with the correction derived from $\mathbf{z}.\mathbf{r}\times\mathbf{k}$ [(4)].

Discussion

Although (6) in general no longer permits a separation of $(\mathrm{d}z/\mathrm{d}s)\Delta s_i$ into an incremental scan step and a Lorentz factor, it does correct for the different velocities of different reciprocal-lattice points through the Ewald sphere. Moreover it offers two distinct advantages over the Lorentz correction hitherto applied to linear scans in reciprocal space.

First, it is completely general. The same analytical form for the correction applies to rotational scans in real space as to linear scans in reciprocal space, as indeed to any type of scan. This affords considerable simplification in the data-reduction program.

Secondly, since the $\Delta\omega_i$, $\Delta\chi_i$ and $\Delta\varphi_i$ used in (6) are the observed steps, it corrects for any known errors in the positioning of successive steps whatever the type of scan. For a linear scan in reciprocal space, equal steps along **q** are usually desired. In practice however the extent to which successive steps Δq_i in a step scan are equal is limited by the mechanical precision of the instrument axes; for many conventional diffractometers the smallest angular step of any axis is 0·01 °. Hence in the conversion from **q** to the setting ω, χ, φ some rounding off of the angles will result, with the consequence that successive steps will be constant in neither Δq_i nor angle. In general the scan performed will not even be linear in reciprocal space. For a rotational scan about one axis, any known irregularities in the size of successive steps are corrected for by the trapezoidal summation, since, all other instrumental angles being fixed, the scan is still carried out along the one arc. For the reciprocal-space scan, however, even if the **q** values corresponding to the actual set angles were calculated and used in the summation of (1) the irregularities in the steps would not be entirely corrected for since the scan performed is no longer linear. Performing the summation over $\lambda\mathbf{z}.\Delta\mathbf{k}_i$ rather than Δq_i corrects completely for missetting of successive steps, since $\lambda\mathbf{z}.\Delta\mathbf{k}_i$ is only sensitive to the distance perpendicular to the Ewald sphere. The same comment applies equally well to flat-cone scans in which the rotation of the levels is accomplished by a combination of angular displacements in ω, χ and φ (Prince, Wlodawer & Santoro, 1978). The trapezoidal summation should be performed over $\lambda\mathbf{z}.\Delta\mathbf{k}_i$ rather than over an angle which does not correspond to a physical axis of the instrument. Note however that use of (6) will not correct for unknown positioning errors. The effect of these on the precision of the structure amplitude has been discussed by Lehmann (1975).

A final caution is that, as with any scan to measure F^2, care must be taken to ensure that the detector is large enough to receive the diffracted beam over the full active range of the reflection. This is particularly so if the trajectory of the scan is not nearly parallel to the long axis of the resolution ellipsoid.

Table 1 presents the observed relative F^2 obtained using (1) and (6) for a number of different types of scans through the 220 reflection of a 3 mm cubic crystal of KD_2PO_4 (DKDP). The scans were made on the four-circle neutron diffractometer D19 at the Institut Laue–Langevin (Thomas, Stansfield, Berneron, Filhol, Greenwood, Jacobé, Feltin & Mason, 1983). This diffractometer is equipped with a large two-dimensional PSD which permits general scans through reflections out of the equatorial plane. Various angular and linear scans were made at $\nu = 0$ and $\nu = 20°$ at a wavelength of 1·55 Å. Although the angles could be read with an accuracy of 0·001°, they could be set only to the closest 0·01°; this is reflected in the root-mean-square deviations of the angular steps, especially for the linear scans. The agreement amongst the F^2 at a particular ν is very good. In general there are two degrees of freedom for the orientation of a particular reflection, choice of ν and rotation around the scattering vector (~choice of φ).

Table 1. *Mean angular and integration steps* (°) *for some angular and linear scans through the* 220 *reflection of DKDP at* (*a*) $\nu = 0°$ *and* (*b*) $\nu = 20°$

'010 scan', for example, denotes a scan along the reciprocal-space direction [010] through the 220 reflection. [ ] contains the root-mean-square deviation in the least significant digits of individual steps from the mean step. The relative counting-statistics error in F^2 is less than 0·1%.

(*a*) Peak maximum at $\gamma = 34·7°$, $\nu = 0°$, $\omega = 17·04°$, $\chi = 180·00°$, $\varphi = -138·42°$

Scan type	$\overline{\Delta\omega}$	$\overline{\Delta\chi}$	$\overline{\Delta\varphi}$	$\overline{\lambda(\mathrm{d}z/\mathrm{d}s)\Delta s}$	F^2
ω scan	0·070 [8]	0	0	−0·039 [5]	213
010 scan	0·022 [7]	0·000 [2]	0·072 [4]	0·028 [6]	213
011 scan	0·022 [8]	−0·108 [7]	0·072 [4]	0·028 [6]	213

(*b*) Peak maximum at $\gamma = 28·18°$, $\nu = 20°$, $\omega = 21·15°$, $\chi = 144·26°$, $\varphi = -138·38°$

Scan type	$\overline{\Delta\omega}$	$\overline{\Delta\chi}$	$\overline{\Delta\varphi}$	$\overline{\lambda(\mathrm{d}z/\mathrm{d}s)\Delta s}$	F^2
ω scan	0·070 [10]	0	0	−0·031 [4]	222
χ scan	0	0·150 [0]	0	−0·019 [0]	224
φ scan	0	0	0·070 [0]	0·038 [0]	223
001 scan	0·000 [5]	−0·217 [10]	0·001 [2]	0·027 [3]	221
010 scan	0·013 [9]	0·052 [4]	0·072 [4]	0·027 [4]	225
011 scan	0·013 [11]	−0·057 [8]	0·072 [4]	0·041 [6]	224

The orientation of the crystal with respect to rotation around the scattering vector was the same for all scans at a particular ν value. The mean path lengths through the crystal are therefore the same for all these scans. This was not the case for the scans at different ν, hence the difference between the average F^2 at the two ν positions.

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On the Statistical Dynamical Theory of Diffraction: Application to Silicon

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Abstract

A detailed solution of Kato's equations describing the propagation of X-rays or neutrons in a crystal containing a statistical distribution of imperfections is presented: this solution makes use of propagation operators to describe multiple scattering events. Corrections to Kato's original solution are given which have a significant effect, even in the case of crystals with a high degree of long-range perfection. The present modified solution is applied to experimental measurement on parallel plates of silicon with different dislocation densities by Olekhnovich, Karpei, Olekhnovich & Puzenkova [*Acta Cryst.* (1983), A**39**, 116-122]. The theory reproduces observations quite well, in contrast to conclusions reached by Olekhnovich *et al.* on the basis of the original solution. It can be inferred that the basic ideas of Kato allow for a correct interpretation of diffraction reflectivities in highly perfect crystals, where a significant contribution from incoherent components of scattered intensities must be incorporated. However, the theory has to be modified for the case of lower long-range perfection: this involves the modification of the expressions for the effective correlation lengths that enter the theory.

I. Introduction

Until 1980, extinction was treated by two very different approaches. Following the ideas of Darwin (1914, 1922), the mosaic model was introduced. In such a model, one considers perfectly coherent multiple scattering within perfect mosaic block, the so-called *primary extinction*, and totally incoherent multiple scattering between adjacent blocks, the so-called *secondary extinction.*

Secondary extinction is therefore described by *energy coupling* equations between the incident and diffracted beams (Zachariasen, 1967; Becker & Coppens, 1974; Kato, 1976), the solution of which is difficult due to the boundary conditions imposed by the sample. Primary extinction, on the other hand, is commonly dealt with through the *amplitude coupling* equations of dynamical theory (Zachariasen, 1945; Batterman & Cole, 1964; Authier, 1970) for perfect crystals.

Mosaic theory is quite popular in crystallography, and has been successfully applied to many practical situations, according in particular to the solution of Becker & Coppens (1974, 1975). Despite this success, it is physically doubtful, since it separates various regions of space discontinuously and arbitrarily. It is clear that distortions from perfect periodicity are much more subtle. A correct model should contain as extreme limits perfect-crystal and mosaic-crystal

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