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Line Profiles for a Collection of Identical Crystals: Effect of a Linear Transformation of Shape

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Abstract

A linear transformation is defined as a distortion of the unit lengths along three Cartesian axes and of their angles, preserving the same covariant coordinates of the corresponding points. The mathematical relationship between the line profiles of two mutually transformed crystals is proposed. It makes it possible, for example, to get the line profiles for ellipsoids, parallelepipeds, distorted tetrahedra and octahedra from the exact results reported by Langford & Wilson [*J. Appl. Cryst.* (1978), **11**, 102–113] for spheres, cubes, regular tetrahedra and octahedra.

The line profile for a collection of identical crystallites of any shape is proportional to

$$I_{hkl}(s) = \frac{1}{U} \int V_{hkl}(t) \cos(2\pi st)\, dt, \qquad (1)$$

where U is the volume of one unit cell, $V_{hkl}(t)$ is the volume common to a crystallite and its 'ghost' shifted a distance t in the direction perpendicular to the reflecting planes hkl, and s is the amount by which the radius vector in reciprocal space, $S = (2 \sin \theta)/\lambda$, exceeds its value for the reciprocal-lattice point hkl (see, for example, Wilson, 1949, p. 41, equation 21). This line profile can be evaluated, in principle, for crystallites of arbitrary shape; the problem reduces to the purely geometrical one of determining $V(t)$ and then finding its cosine Fourier transform. In practice most calculations so far have been confined to regular shapes with cubic or higher symmetry (see Langford & Wilson, 1978, for a survey), though some attention has been given to parallelepipeds (Allegra & Ronca, 1978, 1979) and hexagonal and circular cylinders (Langford, Louër & Wilson, 1980; Langford & Louër, 1982; Louër, Vargas & Langford, 1981). However, as was pointed out by Patterson (1939), results for a regular symmetrical shape may be altered to apply to any non-regular unsymmetrical shapes that can be derived from the regular one by linear transformations of coordinates. Thus results for a cube will lead to those for any parallelepiped, those for a sphere to those for any ellipsoid, and those for a regular tetrahedron or octahedron to those for a non-regular tetrahedron or octahedron. After a linear transformation the new values, $V_1(t_1)$, will be proportional to the old ones, $V(t)$, the proportionality factor being independent of t, and if the crystallite is 'stretched' in the direction of t in the ratio $1:R$, then (1) shows that the line profile as a function of s is simply compressed in the ratio of $R:1$. This conclusion follows even more clearly from an alternative expression for the line profile (Wilson, 1949, p. 35, equation 5), in which the only effect of a linear transformation is to increase all the values of t in the ratio $1:R$. The alternative expression, however, is less convenient for the actual calculation of $I(s)$. For the above regular shapes, except the circular cylinder, $V(t)$ is a cubic in t, and remains so under any linear transformation of coordinates.

We have, therefore, a cubic crystal with unit cell

$$\mathbf{a} = a\mathbf{i}, \quad \mathbf{b} = a\mathbf{j}, \quad \mathbf{c} = a\mathbf{k} \qquad (2)$$

and volume function $V_{hkl}(t)$, and a non-cubic crystal derived from it by a linear transformation and having cell parameters

$$a_1, b_1, c_1; \quad \alpha, \beta, \gamma \qquad (3)$$

and volume function $V_{h_1k_1l_1}(t_1)$ proportional to $V_{hkl}(Rt)$. To make practical use of the results of Langford & Wilson (1978), therefore, it is necessary to determine (i) the pseudo-indices hkl (not necessarily integral) in the cubic crystal corresponding to the indices $h_1k_1l_1$ of the reflection of interest from the non-cubic crystal; and (ii) the value of R.

The *directions* of the reciprocal vectors in the transformed crystal and in the original one (*i.e.* $\mathbf{S}_1$ and

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S respectively) must be related by the same linear transformation holding in direct space. On the other hand, the line profile [see (1)] only depends on the reciprocal direction, which means that the actual lengths $|\mathbf{S}_1|$ and $|\mathbf{S}|$ are unimportant. This leaves us the freedom to select **S** so that it is exactly related to $\mathbf{S}_1$ by the direct-space transformation (Fig. 1). We are thus able to derive $\mathbf{S}(hkl)$ for a given $\mathbf{S}_1(h_1k_1l_1)$, and the problem is solved since $R = |\mathbf{S}_1|/|\mathbf{S}|$, and the pseudo-indices *hkl* are readily obtained. We shall express $\mathbf{S}_1$ and **S** in terms of the components along both the direct ($4a_1$, $4b_1$) and the reciprocal ($4a_2$, $4b_2$) axes, which are coincident for the cubic unit cell:

$$\begin{cases} \mathbf{S}_1(h_1k_1l_1) = x_1^*\,\mathbf{i}_1 + y_1^*\,\mathbf{j}_1 + z_1^*\,\mathbf{k}_1 & (4a_1) \\ \mathbf{S}_1(h_1k_1l_1) = h_1\,\mathbf{a}_1^* + k_1\,\mathbf{b}_1^* + l_1\,\mathbf{c}_1^* & (4a_2) \end{cases}$$

$$\begin{cases} \mathbf{S}(hkl) = x^*\,\mathbf{i} + y^*\,\mathbf{j} + z^*\,\mathbf{k} & (4b_1) \\ \mathbf{S}(hkl) = a^{-1}(h\mathbf{i} + k\mathbf{j} + l\mathbf{k}). & (4b_2) \end{cases}$$

In the above, $\mathbf{i}_1$, $\mathbf{j}_1$, $\mathbf{k}_1$ (**i**,**j**,**k**) are unit vectors along the unit-cell vectors $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ ($a\mathbf{i}$,$a\mathbf{j}$,$a\mathbf{k}$). Further, let p_a, p_b, p_c be the characteristic dimensions of the real crystallite along $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$, while τ is the corresponding common dimension in the regular-shaped crystallite. The required transformation will be given in terms of the dimensions p_a, p_b, p_c and τ, as well as of the lattice parameters of the real crystal. Since ($a_1 = |\mathbf{a}_1|$ *etc.*)

$$\begin{aligned} \mathbf{a}_1\cdot\mathbf{a}_1^* &= a_1(\mathbf{i}_1\cdot\mathbf{a}_1^*) = 1; \\ \mathbf{j}_1\cdot\mathbf{a}_1^* &= \mathbf{k}_1\cdot\mathbf{a}_1^* = 0, \end{aligned} \qquad (5)$$

we may write the following identities (from $4a_1$ and $4b_1$)

$$\frac{a_1}{p_a}\,\mathbf{S}_1(h_1k_1l_1)\cdot\mathbf{a}_1^* = \frac{a_1}{p_a}\,x_1^*(\mathbf{i}_1\cdot\mathbf{a}_1^*) = \frac{x_1^*}{p_a} \qquad (6a)$$

$$\frac{a}{\tau}\,\mathbf{S}(hkl)\cdot\mathbf{a}^* = \frac{x^*}{\tau}. \qquad (6b)$$

Since **S** and $\mathbf{S}_1$ transform according to the deformation tensor of the crystallite, the two above expressions must be identical. Remembering that $a^* = a^{-1}$, we have

$$x^* = ha^* = \frac{h}{a}, \qquad (7)$$

so that, equating (6*a*) to (6*b*), we get

$$h = \frac{\tau}{p_a}\,ax_1^*. \qquad (8)$$

On the other hand, x_1^* is equal to $a_1(\mathbf{S}_1\cdot\mathbf{a}_1^*)$ (*cf.* 6*a*) and the scalar product is conveniently evaluated through ($4a_2$):

$$x_1^* = a_1\,\mathbf{S}_1\cdot\mathbf{a}_1^* = a_1a_1^*q_h, \qquad (9)$$

where

$$\begin{aligned} q_h &= h_1a_1^* + k_1b_1^*\cos\gamma^* + l_1c_1^*\cos\beta^* \\ q_k &= h_1a_1^*\cos\gamma^* + k_1b_1^* + l_1c_1^*\cos\alpha^* \\ q_l &= h_1a_1^*\cos\beta^* + k_1b_1^*\cos\alpha^* + l_1c_1^* \end{aligned} \qquad (9')$$

are quantities already defined in previous papers and denoted as q_1, q_2, q_3 (see, *e.g.* Allegra, Bassi & Meille, 1978). Substitution into (8) gives

$$\begin{aligned} h &= \frac{\tau}{p_a}\,aa_1a_1^*q_h \\ k &= \frac{\tau}{p_b}\,ab_1b_1^*q_k \\ l &= \frac{\tau}{p_c}\,ac_1c_1^*q_l \end{aligned} \qquad (10)$$

$$|\mathbf{S}(hkl)| = \frac{1}{a}\,(h^2 + k^2 + l^2)^{1/2} \qquad (10')$$

and the ratio *R* is given by

$$\begin{aligned} R = {} & |\mathbf{S}_1(hkl)|/|\mathbf{S}(hkl)| \qquad (11) \\ = {} & [(h_1a_1^*)^2 + (k_1b_1^*)^2 + (l_1c_1^*)^2 \\ & + 2(h_1a_1^*)(k_1b_1^*)\cos\gamma^* \\ & + 2(h_1a_1^*)(l_1c_1^*)\cos\beta^* \\ & + 2(k_1b_1^*)(l_1c_1^*)\cos\alpha^*]^{1/2} \\ & \times \{\tau[(a_1a_1^*q_h/p_a)^2 \\ & + (b_1b_1^*q_k/p_b)^2 + (c_1c_1^*q_l/p_c)^2]^{1/2}\}^{-1}. \end{aligned}$$

As a first example, let us specialize the above result to the case of parallelepiped crystals, already considered (Allegra & Ronca, 1979, see Fig. 1). It is easy to show, by comparing equation (3) of Allegra & Ronca (1979) with (10) above, that the following identities apply

$$|h| = \tau a/\bar{u}; \quad |k| = \tau a/\bar{v}; \quad |l| = \tau a/\bar{w}, \qquad (12)$$

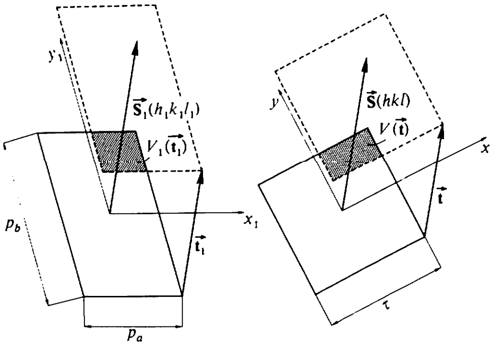

Fig. 1. Relationship between the ideal crystal with cubic symmetry (right) and the real, parallelepiped-shaped crystal obtained after a linear transformation (left). The reciprocal vectors **S** and $\mathbf{S}_1$ are also linearly transformed (see text).

with $\bar{u} = N_h/(a_1^*|q_h|)$, $\bar{v} = N_k/(b_1^*|q_k|)$, $\bar{w} = N_l/(c_1^*/|q_l|)$ (N_h, N_k, N_l are the numbers of unit cells along the crystal edges parallel to $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$), so that the result given by one of us for the cube (see, for example, Wilson, 1949, p. 43, equation 26) is readily converted into equation (1′) of Allegra & Ronca (1979) apart from a factor equal to the unit-cell volume.

Lastly, we shall consider the case of the ellipsoid-shaped crystallite. The line profile of a sphere with radius τ is given by (Langford & Wilson, 1978)

$$I_{hkl}(s) = N\{\psi^{-2} - \psi^{-3}\sin 2\psi + \tfrac{1}{2}\psi^{-4}(1 - \cos 2\psi)\}, \quad (13)$$

where

$$\psi = 2\pi\tau s, \quad (13')$$

and $N = V_{hk}(0)/\mathcal{V}$ is the number of unit cells in the crystal. From the above it readily follows that the diffracted intensity is given by (13) except for the replacement of N with N_1 and of ψ with $2\pi R\tau s$, R being given by (11). p_a, p_b, p_c are here the intercepts of the ellipsoid along three Cartesian axes coinciding with the axes of the unit cell.

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A Technique for the Calculation of Multislice Transmission Functions for Crystals with Large (or Infinite) Repeat Distances in the Beam Direction

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Abstract

A partially analytic technique for the calculation of electron transmission functions used in multislice calculations is developed. This development utilizes the fact that atomic scattering amplitudes are generally available as fitting parameters to four Gaussians. The result is especially applicable to calculations with a large or infinite repeat distance in the incident-beam direction and initial test calculations give a time saving of a factor of four. Sample results are given for the calculation of images from an inclined stacking fault in gold.

Introduction

The multislice method (Cowley & Moodie, 1957; Goodman & Moodie, 1974) for the calculation of dynamical electron scattering has been discussed and used extensively (*e.g.* Bursill & Wilson, 1977; Lynch, 1971).

The object is considered as a series of thin slices with the electron wave function at the exit surface of the nth slice being given by

$$\psi_n(\mathbf{x}) = [\psi_{n-1}(\mathbf{x}) * p_n(\mathbf{x})]\, q_n(\mathbf{x}), \quad (1)$$

where $q_n(\mathbf{x})$ is the transmission function of the nth slice and $p_n(\mathbf{x})$ is the propagation function from the $(n-1)$th to nth slice and $*$ represents the convolution integral. In a typical calculation the distance between slices is chosen to be constant and hence all $p_n(\mathbf{x})$'s are the same and need only be evaluated once and then stored in computer memory.

The transmission function is determined by

$$q_n(x,y\colon z_n,\Delta z) = \exp\{-i\sigma\varphi(x,y\colon z_n,\Delta z)\} \quad (2)$$

(Cowley & Moodie, 1957), where σ is the relativistic interaction constant for electrons and $\varphi(x,y\colon z_n,\Delta z)$ is the projected potential on the x,y plane due to the crystal potential over the thickness Δz from $z = z_n$ to $z_n + \Delta z$. This may be evaluated from the atomic

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