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The Lorentz Factor for the Laue Technique

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Abstract

When the Laue technique is applied to ordinary diffractometer devices and detector systems, problems appear with respect to the Lorentz factor that are unsatisfactorily treated in the literature. A detailed treatment of beam divergence and mosaic spread leads to a derivation of the exact expression for the Lorentz factor for X-ray diffraction with white radiation. This expression differs from the usual formulae if the mosaic spread and beam-divergence angles are of the order of magnitude of the diffraction angle. In addition, the different expressions for the Lorentz factor appearing in the literature are discussed in detail.

Introduction

The discovery of X-ray diffraction by crystals in 1912 (Friedrich, Knipping & von Laue, 1912) led to an exciting development in the field of crystallography. One year later, W. H. Bragg and W. L. Bragg determined the structures of several crystals (Bragg & Bragg, 1913; Bragg, 1913). In the following year, Lorentz derived his Lorentz factor for Laue reflections to calculate structure-factor moduli. Lorentz did not publish his calculations in the traditional way but he informed Debye in a letter about his results. His derivation appears in a note to Debye's paper about the '*Interferenz von Röntgenstrahlen und Wärmebewegung*' (Debye, 1914). This may be the reason why no uniform application of the Lorentz factor for the Laue technique is in use.

Since then, several attempts have been made to derive expressions for the integrated intensity of Laue reflections and the Lorentz factor. From a superficial look at these results, it seems that different expressions are applied. The reasons for this confusion are different definitions and starting points for the calculations. The intention of this paper is:

1. To discuss the effect of mosaic-block distribution and beam divergence on the diffracted intensity in the kinematic approximation. The results of this discussion are used for the derivation of an exact expression for the Lorentz factor.

2. To resolve the confusion with respect to the different formulae given for the Lorentz factor.

Mosaic-block distribution and beam divergence

The process of X-ray diffraction is sensitive to mosaic spread and beam divergence. These quantities influence the diffraction with monochromatic radiation in a different way from white-beam diffraction. The effect of mosaic distribution and beam divergence on diffraction with monochromatic radiation has been treated in detail by Greenhough & Helliwell (1982). These authors derive and discuss general equations for the reflecting range of scattering vectors for oscillation-camera-data processing. From these equations, it is possible to distinguish whether a reflection is fully, partially or not recorded. In the case of partials, the fraction of the reflection can be calculated. Their treatment is based on an oscillating crystal. The basis for the following discussion is a stationary arrangement of beam and crystal.

The presence of constituent crystallites not perfectly aligned within a single crystal is identical to an angular distribution of the scattering vectors. The probability distribution $M(\mathbf{r}_c)$ of the mosaic blocks depends on spherical coordinates $\mathbf{r}_c = (\rho_c, \varphi_c, r_c)$ in reciprocal space fixed to the crystal basis B_c. Let us assume that $M(\mathbf{r}_c)$ is constant within the area F_m and zero outside (Fig. 1):

$$M(\mathbf{r}_c) = \text{constant} \quad \text{for} \quad \mathbf{r}_c = (\rho_c, \varphi_c, r_c) \in F_m$$
and
$$M(\mathbf{r}_c) = 0 \qquad \text{for} \quad \mathbf{r}_c = (\rho_c, \varphi_c, r_c) \notin F_m. \tag{1}$$

F_m is a fragment of a spherical surface with central point at $r_c = 0$ and radius $r_c = |\mathbf{h}| = r_c^h$. The vector $\mathbf{r}_c^b = \mathbf{h}$ is the average direction of all scattering vectors $\mathbf{h}_i$ ending in F_m. Each $\mathbf{h}_i$ represents a single mosaic block of the crystal sample. In a similar way, the divergent incident beam $I_{0M}(\mathbf{r}_l)$ depends on $\mathbf{r}_l = (\rho_l, \varphi_l, r_l)$ in reciprocal space based on the laboratory basis B_l (Fig. 2). $I_{0M}(\mathbf{r}_l)$ follows the conditions

$$I_{0M}(\mathbf{r}_l) = \text{constant} \quad \text{for} \quad \mathbf{r}_l = (\rho_l, \varphi_l, r_l) \in F_i^M$$
and
$$I_{0M}(\mathbf{r}_l) = 0 \qquad \text{for} \quad \mathbf{r}_l = (\rho_l, \varphi_l, r_l) \notin F_i^M. \tag{2}$$

These conditions mean that the intensity in each direction $\mathbf{r}_l$ within F_i^M is constant and that the radiation is absolutely monochromatic with wavelength λ_0. F_i^M is a fragment of a spherical surface with central point at $r_l = 0$ and radius $r_l = 1/\lambda_0 = r_l^{\lambda_0}$.

In general, $M(\mathbf{r}_c)$ is a function of ρ_c and φ_c and the shape of F_i^M depends on the orientation of the crystal sample. $I_{0M}(\mathbf{r}_l)$ can be assumed to be constant for different values of ρ_l and φ_l within F_i^M.

Diffraction with monochromatic radiation

According to the Ewald construction, all $(\rho_l, \varphi_l, r_l^{\lambda_0})$ within F_i^M are central points of Ewald spheres with radii $r_l^{\lambda_0}$. $\mathbf{r}_l^b$ is the average direction of all $\mathbf{r}_l$ within F_i^M.

For further discussion, let us assume that the crystal orientation is near to the ideal Bragg position with respect to $\mathbf{r}_c^b$ and $\mathbf{r}_l^b$. $S_1 = S(\mathbf{r}_l^1)$ is an Ewald sphere with central point at $\mathbf{r}_l^1 = (\rho_l^1, \varphi_l^1, r_l^{\lambda_0})$ within F_i^M and intersects F_m as shown in Figs. 1 and 3(*a*) at $C_1 = C(\mathbf{r}_l^1)$. $S_2 = S(\mathbf{r}_l^2)$ is a second Ewald sphere intersecting F_m at $C_2 = C(\mathbf{r}_l^2)$. Line C_1 crosses line C_2 at $(\rho_c^{12}, \varphi_c^{12}, r_c^h)$. The scattering vector $\mathbf{r}_c^{12} = (\rho_c^{12}, \varphi_c^{12}, r_c^h)$ represents an individual mosaic block of the crystal. This mosaic block is in reflection position simultaneously for the two Ewald spheres S_1 and S_2 taken in this example. From this it can be seen that each scattering vector $\mathbf{r}_c^{ijk\dots} \in F_m$ is simultaneously in diffraction position for several Ewald spheres S_i, S_j, S_k, ... (Fig. 3*b*).

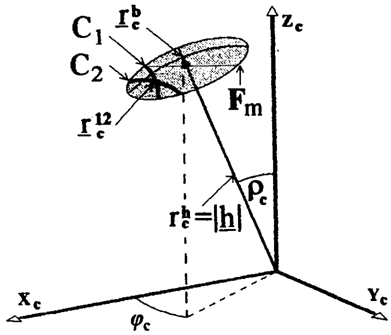

Fig. 1. Reciprocal space with area F_m representing the probability distribution of the mosaic blocks.

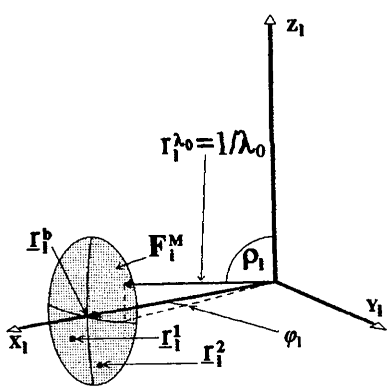

Fig. 2. Reciprocal space with area F_i^M representing the probability distribution of the directions in the incident monochromatic beam.

If the orientations of B_c and B_l are stationary and all possible Ewald spheres within F_i^M are considered, the mosaic blocks within a narrow strip of F_m (Fig. 3*c*) are in diffraction position simultaneously (in this case F_m is large enough and F_i^M comparatively small). The thickness Δs of the strip depends on the angle of the beam divergence $2\beta = \rho_l^{\max} - \rho_l^{\min}$. In order to measure the entire scattered radiation, several neighbouring strips must be collected by changing the relative orientation of B_c with respect to B_l. This procedure is called the 'scan of a reciprocal-lattice vector through the Ewald sphere'.

A scan in equatorial geometry is equivalent to a movement of the crystal perpendicular to the periphery of the strips [direction g in Fig. 3(*c*)]. According to Greenhough & Helliwell (1982), the beam divergence $2\beta = \rho_l^{\max} - \rho_l^{\min}$ and the mosaic spread $2\alpha = \rho_c^{\max} - \rho_c^{\min}$ can be combined to give an effective mosaic spread $\Delta\Omega = 2(\alpha + \beta)$ because both effects have identical reflecting range expressions (equations III.14–III.16 of their treatment). In order to get the total reflection intensity, it is necessary that the sum of n scan intervals δ_i is $\Delta\Omega = \sum_i^n \delta_i$.

The well known Lorentz factor for equatorial geometry and monochromatic radiation (*e.g.* von Laue, 1960) is a consequence of the different passing velocities of scattering vectors through the Ewald-sphere surface during the scans:

$$L_M = \lambda^3/\sin 2\theta. \tag{3}$$

This Lorentz factor can also be applied to stationary measurements with monochromatic radiation: The divergence area F_i^M must be large enough so that not only a narrow strip of F_m but all scattering vectors within F_m are simultaneously in diffraction position. This special case is different from the treatment of Greenhough & Helliwell (1982) because no movement of the crystal is necessary to get the full reflection intensity.

Buras & Gerward (1975) discussed the relations between integrated intensities in monochromatic and polychromatic diffraction methods. Table 1 of their paper contains no Lorentz factor for a stationary single crystal and monochromatic radiation (method *A*2). According to

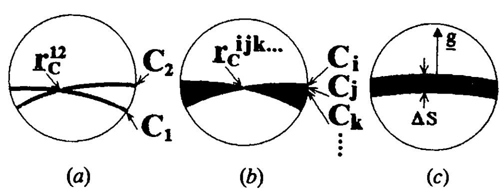

Fig. 3. Lines of intersection of two (*a*) and several (*b* and *c*) Ewald spheres with F_m.

these authors, no integration is possible in this method. In contrast, the angular opening of the incident beam is taken into consideration in the calculations of Kalman (1979). His result is that the Lorentz factors of method (II-1) (monochromatic radiation and stationary crystal) and method (II-2) (monochromatic radiation and rotating crystal) are identical (for $\Psi = 0$, *i.e.* equatorial geometry). This result will be used for the derivation of the Lorentz factor for polychromatic radiation.

Diffraction with white radiation

In order to discuss the geometric conditions for white-beam diffraction, definition (2) of the beam divergence $I_{0M}(\mathbf{r}_l)$ has to be extended in so far that the radial component r_l is variable and not fixed to $r_l = 1/\lambda_0 = r_l^{\lambda_0}$. So F_i^M of a monochromatic beam will be replaced by a volume V_i of a polychromatic beam with radial component $1/\lambda_{\max} \leq r_l = r_l^{\lambda_x} \leq 1/\lambda_{\min}$:

$$I_{0L}(\mathbf{r}_l) = \text{constant} \quad \text{for} \quad \mathbf{r}_l = (\rho_l, \varphi_l, r_l) \in V_i$$

and (4)

$$I_{0L}(\mathbf{r}_l) = 0 \qquad \text{for} \quad \mathbf{r}_l = (\rho_l, \varphi_l, r_l) \notin V_i.$$

The condition of constant intensity $I_{0L}(\mathbf{r}_l)$ within V_i is a simplifying assumption. All (ρ_l, φ_l, r_l) within V_i are possible central points of Ewald spheres with radii $r_l^{\lambda_x} = 1/\lambda_x$ (Fig. 4). Only a small part V_i^L of V_i is selected by the distribution of the scattering vectors within F_m for the diffraction process (Fig. 5).

The mosaic distribution, in combination with the divergence of the incident beam, selects a subinterval of wavelengths $[\lambda^h_{\min}, \lambda^h_{\max}]$ determining the wavelength distribution of the Laue reflection. This subinterval will be calculated later.

The smaller the mosaic spread 2α and the beam divergence 2β (Fig. 5 and Appendix), the smaller is $[\lambda^h_{\min}, \lambda^h_{\max}]$. Also, the radial angular spread Φ of a reflection depends on α and β. In general, $\Phi = 2(2\alpha + 2\beta)$. If synchrotron radiation is used, the beam divergence is $2\beta \simeq 0$. In this case, the spread of the reflection is $\Phi \simeq 4\alpha$. Andrews, Hails, Harding & Cruickshank (1987) reported on the observed effect of mosaic spread on Laue spot profiles and their interpretation.

In order to satisfy the diffraction condition for a scattering vector $\mathbf{r}_c \in F_m$, a plane P_c perpendicular to $\mathbf{r}_c$ must be constructed in such a way that P_c intersects $\mathbf{r}_c$ at $\mathbf{r}_c/2$. According to the Ewald construction, each $(\rho_c, \varphi_c, r_c) \in P_c$ is a possible central point of an Ewald sphere. The entire volume $V_i^L \in V_i$ that is selected for the diffraction process consists of all $\mathbf{p}_c = (\rho_c, \varphi_c, r_c)$ following the condition

$$V_i^L = \{\mathbf{p}_c = (\rho_c, \varphi_c, r_c)\}: \quad \mathbf{p}_c \in P_c \wedge \mathbf{p}_c \in V_i$$

with

$$P_c \perp \mathbf{r}_c \wedge \mathbf{r}_c \in F_m \wedge \tfrac{1}{2}\mathbf{r}_c \in P_c. \tag{5}$$

V_i^L is the part with dark shading in Fig. 5; in the light part of V_i, the diffraction condition cannot be satisfied.

From now on, monochromatic and white-beam diffraction for a stationary arrangement of beam and crystal are compared with each other. If F_i^M of the monochromatic beam is large enough, the total area F_m and, consequently, all mosaic blocks are simultaneously in diffraction position. The integrated intensity I_M can be recorded by a single measurement as a consequence. Let us consider that F_i^M has a 'thickness' $\mathrm{d}s = \mathrm{d}(1/\lambda)$, *i.e.* that the radiation has an infinitesimal bandwidth. Each volume element $\mathrm{d}V_i^M = \mathrm{d}F_i^M \mathrm{d}s \in F_i^M \mathrm{d}s = V_i^M$ contains the central point of an Ewald sphere satisfying the Bragg condition. The number N^M of these volume elements is proportional to the square of the radius of the Ewald spheres $(1/\lambda)^2$: $N^M \propto V_i^M \propto F_i^M \propto 1/\lambda^2$.

The same considerations are valid for white-beam diffraction. Each volume element $\mathrm{d}V_i^L \in V_i^L$ contains the central part of an Ewald sphere satisfying the Bragg condition (Fig. 5). The total integrated intensity I_L results from V_i^L. The number N^L of these Ewald spheres is proportional to V_i^L. Some simple geometric relations lead to the result (see Appendix) that $V_i^L \propto 1/(\lambda^3 \tan\theta) \propto (|\mathbf{h}|^3 \cos\theta)/\sin^4\theta$.

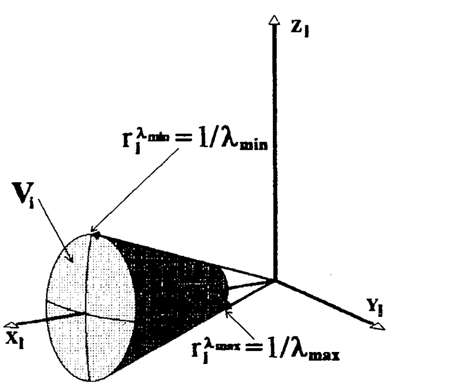

Fig. 4. V_i from a polychromatic incident beam with divergence.

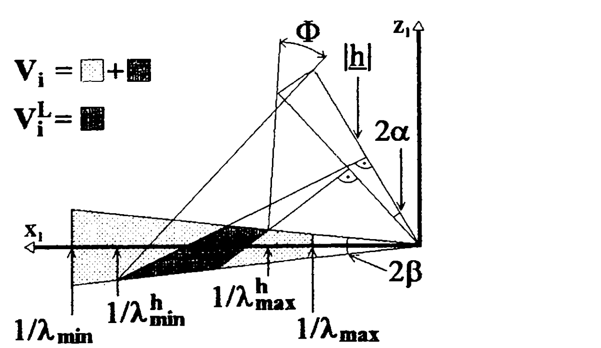

Fig. 5. Within V_i^L, the Bragg condition is satisfied. 2α is the mosaic angle and 2β the angle of beam divergence.

The quotients V_i^L/V_i^M and N^L/N^M are proportional to the quotient of the integrated intensities $I_L = |F|^2 L_L P_L I_{0L}$ and $I_M = |F|^2 L_M P_M I_{0M}$:

$$\begin{aligned} N^L/N^M &\propto V_i^L/V_i^M \\ &\propto I_L/I_M \\ &\propto |F|^2 L_L P_L I_{0L}/(|F|^2 L_M P_M I_{0M}) \\ &\propto L_L/L_M. \end{aligned} \tag{6}$$

The polarization factor P_L is equal to P_M for unpolarized radiation. Therefore, V_i^L/V_i^M is proportional to the quotient of both Lorentz factors L_L and L_M. With the proportional constant set to unity, the Lorentz factor L_L for white-beam diffraction may be written

$$\begin{aligned} L_L &= L_M(V_i^L/V_i^M) \\ &= L_M/[1/(\lambda^3 \tan\theta)]/(1/\lambda^2) \\ &= (\lambda^3/\sin 2\theta)\cos\theta/(\lambda \sin\theta) \\ &= \lambda^2/\sin^2\theta. \end{aligned} \tag{7}$$

Exact expression for the Lorentz factor

The previous derivation of the Lorentz factor (7) is based on two approximations (see Appendix): 2α and $2\beta \ll \theta$. This assumption is normally permitted. Otherwise, an exact expression for the Lorentz factor has to be used.

If synchrotron sources are used for single-crystal data collection by the Laue technique (*e.g.* Bartunik & Borchert, 1989; Helliwell, Gomez de Anderez, Habash, Helliwell & Vernon, 1989), the properties of the radiation and the large distance between source and crystal lead to a practically vanishing divergence $2\beta \simeq 0$. Consequently, the exact Lorentz factor is needed for $2\alpha \simeq \theta$.

The Laue diffractometer used by the author (Lange & Burzlaff, 1992, 1995) works with a conventional tungsten X-ray tube. The present tube–crystal distance is set to 160 mm. This short distance between tube and crystal is necessary to obtain sufficient intensity for single-crystal data collections with an accuracy comparable to the monochromatic technique. The X-ray tube that is in use is a Siemens type FK 60-04 W with a focal-spot size of 0.4×0.8 mm and a working voltage of 50 kV. A medium-sized single-crystal sample of about 0.6 mm diameter leads to a divergence angle $2\beta = 0.50°$. If a reciprocal-lattice vector $\mathbf{h}$ is in diffraction position at a short wavelength, the value of the Bragg angle θ can have the same order of magnitude as 2α and 2β. In this case, the approximation α and $\beta \to 0$ leads to deviations using the Lorentz factor (7).

To get the exact expression (9) for the Lorentz factor, $1/(\lambda^3 \tan\theta)$ in (7) is replaced by relation (27) of the Appendix:

$$\begin{aligned} V_i^L \propto |\mathbf{h}|^3 \{&\sin(\theta-\alpha)/[\sin^2(\theta-\alpha+\beta) \\ &\times \sin^2(\theta-\alpha-\beta)] \\ &- \sin(\theta+\alpha)/[\sin^2(\theta+\alpha+\beta) \\ &\times \sin^2(\theta+\alpha-\beta)]\}, \end{aligned} \tag{8}$$

which leads to

$$\begin{aligned} L_L = \lambda^2 \sin^2\theta/\cos\theta \\ \times \{&\sin(\theta-\alpha)/[\sin^2(\theta-\alpha+\beta)\sin^2(\theta-\alpha-\beta)] \\ &- \sin(\theta+\alpha)/[\sin^2(\theta+\alpha+\beta)\sin^2(\theta+\alpha-\beta)]\}. \end{aligned} \tag{9}$$

Tables 1 and 2 show the dependence of $D(\theta)$ on the Bragg angle θ. The normalized quantity $D(\theta)$ is the quotient of the exact Lorentz factor L_{exact} (9) and L_{approx} (7) multiplied by a normalization factor N:

$$D(\theta) = (L_{\text{exact}}/L_{\text{approx}})N$$

with

$$N = \lim_{\alpha,\beta\to 0}(L_{\text{approx}}/L_{\text{exact}}) = \text{constant},$$

so that

$$\lim_{\alpha,\beta\to 0} D(\theta) = 1. \tag{10}$$

Table 2 shows that the quotient of L_{exact} and L_{approx} increases rapidly with decreasing θ. The author intends to verify his calculations with the Laue diffractometer experimentally. These experiments are difficult since the signal-to-background ratio is poor for small diffraction angles. Furthermore, the wavelength distribution of the white radiation must be well known.

Discussion of the Lorentz factor

The modulus of the structure factor $|F(\mathbf{h})|$ can be derived from the integrated intensity $\tilde{I}(\lambda,\mathbf{h})$ in the kinematical approximation with the assumption of negligible crystal sample absorption by

$$\tilde{I}(\lambda,\mathbf{h}) \propto |F(\mathbf{h})|^2 PL(\lambda,\theta)\tilde{I}_0(\lambda). \tag{11}$$

$L(\lambda,\theta)$ is the Lorentz factor and P the polarization factor. Three different proposals for the Lorentz factor can be found:

1. $L = \lambda^2/\sin^2\theta$ (*e.g.* von Laue, 1926; Lorentz, cited in Debye, 1914);
2. $L = \lambda^3/\sin^2\theta$ (*e.g.* Gonschorek, 1983);
3. $L = \lambda^4/\sin^2\theta$ (*e.g.* Rabinovich & Lourie, 1987; Zachariasen, 1945).

These formulae seem to be contradictory. A critical comparison of the different papers, however, shows that these discrepancies result from a different use of the terms 'integrated intensity' $\tilde{I}(\lambda,\mathbf{h})$ and 'intensity of the incident beam' $\tilde{I}_0(\lambda)$ by the authors. This problem is briefly discussed in the paper by Kalman (1979). The

Table 1. *Parameters*

Parameter	Example 1	Example 2
2α (°)	0.15	0.30
2β (°)	0.50	0.50
$\lvert\mathbf{h}\rvert$ (Å^{-1})	0.10	0.07
Tube voltage (kV)	50	50

Table 2. *Calculated values for* $D(\theta)$

Example 1				Example 2			
θ(°)	$D(\theta)$	λ (Å)	E (keV)	θ(°)	$D(\theta)$	λ (Å)	E (keV)
				0.75	1.82	0.37	33.2
				1.00	1.36	0.50	24.9
1.25	1.16	0.29	42.6	1.25	1.21	0.62	19.9
1.50	1.11	0.35	35.5	1.50	1.14	0.75	16.6
2.00	1.06	0.47	26.6	2.00	1.07	1.00	12.4
3.00	1.03	0.70	17.8	3.00	1.03	1.50	8.3
4.00	1.01	0.93	13.3	4.00	1.02	2.00	6.2
7.00	1.00	1.63	7.6	7.00	1.01	3.50	3.6

discrepancies vanish if the terms are correctly defined and used for the discussion.

Relation (11) can be written in greater detail:

$$N(\lambda)/\Delta\lambda_{\mathbf{h}} \propto |F(\mathbf{h})|^2 P(\lambda^2/\sin^2\theta)[N_0(\lambda)/\Delta\lambda]. \quad (12)$$

$N(\lambda)$ is the number of counted photons of the selected reflection $F(\mathbf{h})$ within the interval $\Delta\lambda_{\mathbf{h}}$. The quantity $\Delta\lambda_{\mathbf{h}}$ is the interval that is selected by the scattering vector $\mathbf{h}$. It depends on $|\mathbf{h}|$, λ and the mosaic spread [see (16)]. $N_0(\lambda)$ is the number of photons in the incident beam within the interval $\Delta\lambda$, which is a fixed interval. With the transformation relation

$$\Delta E = \hbar\Delta\omega = |\mathrm{d}E/\mathrm{d}\lambda|\Delta\lambda = (hc/\lambda^2)\Delta\lambda, \quad (13)$$

(12) can be changed to

$$N(\lambda)/\Delta E_{\mathbf{h}} \propto |F(\mathbf{h})|^2 P(\lambda^4/\sin^2\theta)[N_0(\lambda)/\Delta\lambda]. \quad (14)$$

If $N(\lambda)/\Delta E_{\mathbf{h}}$ is used, the expression $\lambda^4/\sin^2\theta$ appears and is also called the 'Lorentz factor' in the literature. Multiplying (14) with energy E, one obtains an integrated intensity $\tilde{I}$ per interval $\Delta E_{\mathbf{h}}$:

$$\begin{aligned}\tilde{I}/\Delta E_{\mathbf{h}} &= [N(\lambda)/\Delta E_{\mathbf{h}}]E \\ &\propto |F(\mathbf{h})|^2 P(\lambda^3/\sin^2\theta)[N_0(\lambda)/\Delta\lambda]. \quad (15)\end{aligned}$$

The factor $\lambda^3/\sin^2\theta$ in (15) is also falsely called the 'Lorentz factor' when it is used in this way. $N_0(\lambda)/\Delta\lambda$ appearing in (12), (14) and (15) is not the 'intensity of the incident beam' but the number of incident photons $N_0(\lambda)$ within $\Delta\lambda$.

The choice of one of these expressions depends on the interpretation of the measured data:

1. The wavelength interval $\Delta\lambda_{\mathbf{h}} = [\lambda^h_{\min}, \lambda^h_{\max}]$ is selected by the effective mosaic spread. The effective mosaic spread is the sum of the mosaic spread 2α and the beam divergence 2β, $\Delta\Omega = 2(\alpha+\beta)$ (notice that $\Delta\Omega \neq \Phi$). With the Bragg equation, $\Delta\lambda_{\mathbf{h}}$ is

$$\begin{aligned}\Delta\lambda_{\mathbf{h}} &= 2(\cos\theta/|\mathbf{h}|)\Delta\Omega \\ &= (2\Delta\Omega/|\mathbf{h}|)\cos\{\arcsin[(|\mathbf{h}|/2)\lambda]\}. \quad (16)\end{aligned}$$

N and λ of a Laue reflection can be determined using an energy-resolving detector. $N_0(\lambda)/\Delta\lambda$ of the incident beam for X-ray tube *Bremsstrahlung* can be taken from *International Tables for Crystallography* (1992) and Kramers (1923). From these values and the Lorentz factor $\lambda^2/\sin^2\theta$, $|F(\mathbf{h})|$ can be calculated by (12).

2. Converting (16) by using (13) so that $\Delta E_{\mathbf{h}}$ is a function of $\Delta\Omega$ then (14) is the correct equation.

3. Formula (15) is the correct relation if $N/\Delta E_{\mathbf{h}}$ is multiplied by E of the reflection or when a detector system is used that directly measures a quantity proportional to the total energy $N(\lambda)E$ (*e.g.* Blank, Burzlaff & Hümmer, 1982).

The results of the previous discussion are summarized: different expressions for the Lorentz factor [(12), (14) and (15)] exist. In the literature, these expressions are applied in the way previously described. This is why some authors obtain reasonable results although they do not always know why they have to apply a special 'Lorentz factor'.

Relation (12) is the only one containing the quantities $N_0(\lambda)/\Delta\lambda$ and $N(\lambda)/\Delta\lambda_{\mathbf{h}}$, which have the same physical meaning. The expressions for the primary and the secondary beams are different in (14) and (15). One can convert (14) and (15) using (13) so that the expressions for the primary and the secondary beams also have the same physical meaning.

Equation (14) leads to

$$N(\lambda)/\Delta E_{\mathbf{h}} \propto |F(\mathbf{h})|^2 P(\lambda^2/\sin^2\theta)\{\lambda^2[N_0(\lambda)/\Delta\lambda]\}$$

with

$$\lambda^2[N_0(\lambda)/\Delta\lambda] = hc[N_0(\lambda)/\Delta E] \propto N_0(\lambda)/\Delta E. \quad (17)$$

Equation (15) leads to

$$[N(\lambda)/\Delta E_{\mathbf{h}}]E \propto |F(\mathbf{h})|^2 P(\lambda^2/\sin^2\theta)\{\lambda[N_0(\lambda)/\Delta\lambda]\}$$

with

$$\lambda[N_0(\lambda)/\Delta\lambda] = [N_0(\lambda)/\Delta E]E. \quad (18)$$

Lorentz derived his factor as a geometric correction factor. The additional quantities λ^2 in (17) and λ in (18) are not a part of the Lorentz factor but a consequence of the different representations of the primary and the secondary beams. Only the expression $\lambda^2/\sin^2\theta$ is the real Lorentz factor in accordance with the intention of H. A. Lorentz. The other factors consist of the Lorentz factor and the additional quantities λ and λ^2.

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APPENDIX
Derivation of the volume V_i^L

It is not necessary for the derivation of V_i^L that the basis area of the cone has a circular shape as shown in Fig. 4. In reality, the shape depends on the orientation of the crystal. Any shape can be assembled by infinitesimal squares. So it is sufficient to calculate V_i^h for a pyramidal cone with quadratic basic area. Necessary parameters for the derivation are shown in Fig. 6 and given by the following equations:

$$\begin{aligned} a_1 &= |\mathbf{h}|/[2\sin(\theta+\alpha-\beta)],\\ a_2 &= |\mathbf{h}|/[2\sin(\theta-\alpha-\beta)], \end{aligned} \tag{19}$$

$$\begin{aligned} b_1 &= 2a_1\tan\beta = |\mathbf{h}|\tan\beta/\sin(\theta+\alpha-\beta),\\ b_2 &= 2a_2\tan\beta = |\mathbf{h}|\tan\beta/\sin(\theta-\alpha-\beta), \end{aligned} \tag{20}$$

$$\begin{aligned} c_1 &= |\mathbf{h}|/[2\sin(\theta+\alpha+\beta)],\\ c_2 &= |\mathbf{h}|/[2\sin(\theta-\alpha+\beta)], \end{aligned} \tag{21}$$

$$\begin{aligned} d_1 &= 2c_1\tan\beta = |\mathbf{h}|\tan\beta/\sin(\theta+\alpha+\beta),\\ d_2 &= 2c_2\tan\beta = |\mathbf{h}|\tan\beta/\sin(\theta-\alpha+\beta), \end{aligned} \tag{22}$$

$$\begin{aligned} e_1 &= |\mathbf{h}|\sin(2\beta)/[2\sin(\theta+\alpha+\beta)\sin(\theta+\alpha-\beta)],\\ e_2 &= |\mathbf{h}|\sin(2\beta)/[2\sin(\theta-\alpha+\beta)\sin(\theta-\alpha-\beta)]. \end{aligned} \tag{23}$$

θ is the Bragg angle, 2α the angle of the mosaic spread, 2β the beam divergence angle and $|\mathbf{h}|$ the modulus of the reciprocal-lattice vector. The volume of a cone is $V = 1/3\,GH$. G is the basis area and H is the height of the cone perpendicular to G. The resulting volume ΔV is

$$\Delta V = \tfrac{1}{3}H(G_2 - G_1) = (|\mathbf{h}|/6)(G_2 - G_1). \tag{24}$$

The perpendicular height of both cones is $|\mathbf{h}|/2$ and the basis areas are G_1 and G_2. In the following, G_2 is calculated in detail:

$$\begin{aligned} G_2 &= (d_2/2 + b_2/2)e_2\\ &= [1/\sin(\theta-\alpha+\beta) + 1/\sin(\theta-\alpha-\beta)]\\ &\quad\times\left[\frac{|\mathbf{h}|^2\tan\beta\sin(2\beta)}{4\sin(\theta-\alpha+\beta)\sin(\theta-\alpha-\beta)}\right]\\ &= \left[\frac{\sin(\theta-\alpha-\beta)+\sin(\theta-\alpha+\beta)}{\sin^2(\theta-\alpha+\beta)\sin^2(\theta-\alpha-\beta)}\right]\\ &\quad\times|\mathbf{h}|^2\tan\beta\sin(2\beta)/4\\ &= \left[\frac{\sin(\theta-\alpha)\cos\beta}{\sin^2(\theta-\alpha+\beta)\sin^2(\theta-\alpha-\beta)}\right]\\ &\quad\times|\mathbf{h}|^2\tan\beta\sin(2\beta)/2. \end{aligned} \tag{25}$$

The calculation for G_1 yields

$$\begin{aligned} G_1 &= \left[\frac{\sin(\theta+\alpha)\cos\beta}{\sin^2(\theta+\alpha+\beta)\sin^2(\theta+\alpha-\beta)}\right]\\ &\quad\times|\mathbf{h}|^2\tan\beta\sin(2\beta)/2. \end{aligned} \tag{26}$$

The resulting volume ΔV is

$$\begin{aligned} \Delta V \propto |\mathbf{h}|^3&\left[\frac{\sin(\theta-\alpha)}{\sin^2(\theta-\alpha+\beta)\sin^2(\theta-\alpha-\beta)}\right.\\ &\left.-\frac{\sin(\theta+\alpha)}{\sin^2(\theta+\alpha+\beta)\sin^2(\theta+\alpha-\beta)}\right]. \end{aligned} \tag{27}$$

For $2\beta \ll \theta$, ΔV is approximately

$$\begin{aligned} \lim_{\beta\to 0}\Delta V &\propto |\mathbf{h}|^3[\sin(\theta-\alpha)\sin^4(\theta+\alpha)\\ &\quad-\sin(\theta+\alpha)\sin^4(\theta-\alpha)]\\ &\quad\times[\sin^4(\theta+\alpha)\sin^4(\theta-\alpha)]^{-1}\\ &= 8|\mathbf{h}|^3\{[\sin^3(\theta+\alpha)-\sin^3(\theta-\alpha)]\\ &\quad\times[\cos(2\alpha)-\cos(2\theta)]^{-3}\}\\ &= 2|\mathbf{h}|^3\{[3\sin(\theta+\alpha)-\sin(3\theta+3\alpha)\\ &\quad-3\sin(\theta-\alpha)+\sin(3\theta-3\alpha)]\\ &\quad\times[\cos(2\alpha)-\cos(2\theta)]^{-3}\}\\ &= 2|\mathbf{h}|^3\{[6\cos\theta\sin\alpha-2\cos(3\theta)\sin(3\alpha)]\\ &\quad\times[\cos(2\alpha)-\cos(2\theta)]^{-3}\}. \end{aligned} \tag{28}$$

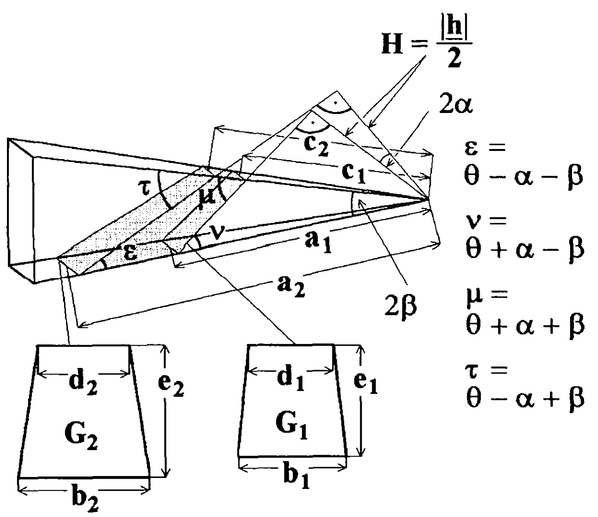

Fig. 6. Parameters for the derivation of V_i^L.

The next approximation $2\alpha \to 0$ leads to the final result for ΔV:

$$\begin{aligned}\lim_{\beta,\alpha\to 0} \Delta V &\propto |\mathbf{h}|^3 6 \sin\alpha[\cos\theta - \cos(3\theta)]/\sin^6\theta \\ &\propto |\mathbf{h}|^3 6\alpha[\cos\theta - \cos(3\theta)]/\sin^6\theta \\ &\propto |\mathbf{h}|^3[\cos\theta/\sin^4\theta] \\ &\propto 1/(\lambda^3 \tan\theta). \qquad (29)\end{aligned}$$

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Statistical Descriptors in Crystallography. II.

Report of a Working Group* on Expression of Uncertainty in Measurement

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Abstract

The Working Group has examined recent recommendations for evaluating and expressing uncertainty in measurement [*Guide to the Expression of Uncertainty in Measurement*, International Organization for Standardization (ISO, 1993)]. The present publication updates an earlier report of the IUCr Subcommittee on Statistical Descriptors [Schwarzenbach, Abrahams, Flack, Gonschorek, Hahn, Huml, Marsh, Prince, Robertson, Rollett & Wilson (1989). *Acta Cryst.* A**45**, 63–75]. This new report presents the concepts of standard uncertainty, of combined standard uncertainty, and of Type A and Type B evaluations of standard uncertainties. It expands the earlier dictionary of statistical terms, recommends replacement of the term *estimated standard deviation* (e.s.d.) by *standard uncertainty* (s.u.) or by *combined standard uncertainty* (c.s.u.) in statements of the statistical uncertainties of data and results, and requests a complete description of the experimental and computational procedures used to obtain all results submitted to IUCr publications.

Introduction

The International Organization for Standardization (ISO) has issued a document (ISO, 1993), hereafter referred to as *Guide*, with the purpose of establishing general rules for evaluating and expressing the uncertainty of the result of a measurement. Based on a recommendation of the Comité International des Poids et Mesures, the rules are intended to be applicable to a broad spectrum of measurements. A recent NIST Technical Note (Taylor

* Appointed 4 March 1993 as a Working Group of the International Union of Crystallography Commission on Crystallographic Nomenclature. The final report of the Working Group was accepted on 20 September 1994 by the Commission and 15 December 1994 by the Executive Committee.

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