

calculated using the experimentally determined elastic constants and are shown in Fig. 5 where the dotted curves are corrected for second-order diffuse reflexion and the solid curves are without this correction. The variation of second-order correction with direction can be seen from Fig. 5.

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Absorption and Volume Corrections for a Cylindrical Specimen, Larger than the Beam, and in General Orientation

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A theory and a computer procedure are developed by which both the absorption and the volume corrections for a cylindrical sample of infinite length, larger than the beam, enclosed in a concentric cylindrical tube, and in general orientation in the Eulerian cradle, can be carried out. The combined corrections can be used in the simpler case of an exposed sample. Moreover, the absorption correction can be applied to the case of a cylindrical window, such as may be employed in low-temperature studies, surrounding a sample of conventional size.

A theory for both the absorption and volume corrections for a cylindrical specimen, larger than the beam, and whose axis is coincident with the φ -axis of the goniometer, is given in an earlier paper (Coyle & Schroeder, 1971). In the present paper, an extension of that theory is developed for the case of a similar specimen, but in general orientation. The two corrections for such a crystal are available as computer program *CYCAC*.

The same terminology and symbols are followed here, but additional independent angles are defined for the sake of convenience and in such a way as to obtain equations algebraically symmetrical to those of the earlier paper.

Let Γ , where $0 \leq \Gamma \leq \pi/2$, be the angle between the crystal axis J and the φ axis of the diffractometer. If Γ is less than, or equal to, the maximum possible arc settings (the usual case), it is given by $\cos \Gamma = \cos \gamma_i \cos \gamma_o$, where γ_i and γ_o are the inner and outer arc setting differences required to bring the two axes into coincidence.

Furthermore, let the χ circle be a great circle of a

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sphere centered on the goniometer with the zero of χ at the south pole S , and let the fiducial zero of φ be that value of φ when Γ lies in the great χ circle in a positive χ direction. Let the positive sense of φ be counter-clockwise when viewed from the center, and the positive sense of χ be toward the point E , where the diffraction vector \mathbf{h} for positive Bragg angle θ meets the sphere. In the diffraction position, let the crystal axis J meet the great circle through S a spherical distance χ_1 from S , and let this great circle meet the equator in E_1 , a spherical distance β from E .

Then, as in Fig. 1, the oblique spherical triangle $\chi\chi_1\Gamma$ yields:

$$\cos \chi_1 = \cos \chi \cos \Gamma - \sin \chi \sin \Gamma \cos \varphi.$$

Strictly speaking, this relationship is true only if $\varphi \leq \pi$, but of course the crystal axis meets the sphere in two diametrically opposed points and we require for computation not $\sin \chi_1$ and $\cos \chi_1$ themselves, but their squares.

Also, since EE_1S is a biquadrantal triangle, β is also the angle $E\hat{S}E_1$ and $\tan \beta = \sin \Gamma \sin \varphi / (\sin \Gamma \cos \chi \cos \varphi + \sin \chi \cos \Gamma)$. Computationally, β appears positive in the first and third quadrants and negative in the second and fourth, and is computed as its principal value from either pole.

The absorption and volume correction factors may be derived in a similar fashion to the method given earlier. The variables are merely modified. Thus, χ in the earlier equations is always replaced with χ_1 , while θ sometimes remains, and at other times is replaced with $(\theta \pm \beta)$. Indeed, all relationship derived here must degenerate to those given earlier ($\Gamma=0$) by putting $\chi_1=\chi$ and $\beta=0$.

Fig. 2 presents the elliptical cross-section in the diffraction plane of the sample cylinder, whose canonical equation is $x^2 + y^2 \cos^2 \chi_1 = R^2$. This figure is similar to Fig. 2 in the earlier paper, except that now reflection is equiangular to the diameter inclined at the angle β to the minor axis. The volume correction is now given by:

$$I^0/I_0^0 = \rho/R = (1 - \sin^2(\theta - \beta) \sin^2 \chi_1)^{-1/2}. \quad (1)$$

In the derivation of the absorption correction factor, the coefficients in the expression for the outgoing elliptical radius $A\sigma^4 + B\sigma^2 + C = 0$ now become:

$$\begin{aligned} A &= [1 - \sin^2(\theta + \beta) \sin^2 \chi_1]^2, \\ B &= -2R^2[1 - \sin^2(\theta + \beta) \sin^2 \chi_1 \\ &\quad - 2(\rho - z)[\cos^2(\theta + \beta) - \sin^2(\theta + \beta) \\ &\quad \times \cos^2 \chi_1] \sin^2 2\theta \sin^2 \chi_1, \\ C &= R^4 + 2R^2(\rho - z)^2 \sin^2 2\theta \sin^2 \chi_1 \cos 2(\theta + \beta) \\ &\quad + (\rho - z)^4 \sin^4 2\theta \sin^4 \chi_1. \end{aligned}$$

The following points may be of special interest.

(a) The roots of the quadratic in σ^2 are always real for reflexion from within the crystal (*i.e.* from physically

plausible points) since:

$$\frac{\rho - z}{\rho} \leq \frac{1 - \sin^2(\theta + \beta) \sin^2 \chi_1}{\sin 2\theta \cos \chi_1}, \quad (2)$$

which has a maximum value of unity. This occurs when $\cos \chi_1 = \pm \cot(\theta + \beta)$, and can occur only when $\theta + \beta \geq \pi/4$. Likewise, the roots are always positive, since $A, C > 0$ and $B < 0$.

- (b) When $z = \rho$, reflection occurs from the center, the roots are equal, and $\sigma^2 = R^2/[1 - \sin^2(\theta + \beta) \sin^2 \chi_1]$.
(c) When $\theta = -\beta$, then even for $\rho \neq z$ the roots are equal and $\sigma^2 = R^2 + (\rho - z)^2 \sin^2 2\theta \sin^2 \chi_1$. In this case the emergent ray is parallel to an axis of the ellipse.
(d) When $\beta > 0$, the larger value of σ is relevant to reflexion before the center when $\theta > |\beta|$, and the smaller root is relevant to reflexion an equal distance beyond the center. The opposite is true

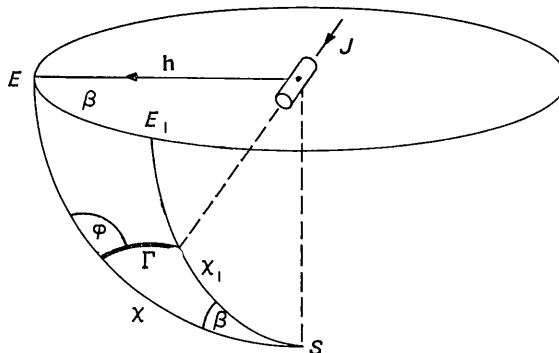


Fig. 1. The experimental arrangement, showing the specimen in position for diffraction and the pertinent spherical angles.

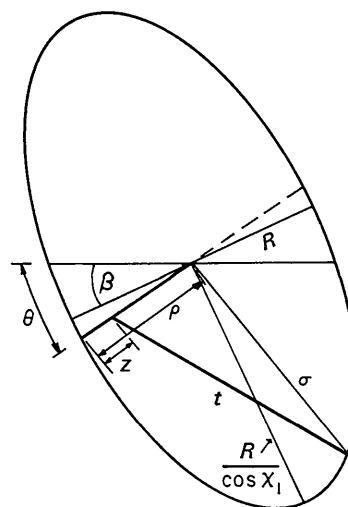


Fig. 2. The elliptical cross-section of the sample cylinder in the diffraction plane. Here z and t are the respective incoming and outgoing path lengths.

when either, but not both, of these inequalities is reversed.

The expression for the emergent path length $t(\sigma, \varrho, z, \theta)$ remains unchanged, so that the overall correction factor for both effects now becomes, for N Gaussian points x_i and their corresponding weights w_i , and for a sample (subscript 1) enclosed in a tube (subscript 2):

$$I/I_0^0 = \frac{1}{2}(1 - \sin^2(\theta - \beta) \sin^2 \chi_1)^{-1/2} \cdot \\ \times \sum_{i=1}^N w_i \exp[-\mu_1(\varrho_1 x_i + \varrho_1 + t_1) \\ - \mu_2(\varrho_2 - \varrho_1 + t_2 - t_1)], \quad (3)$$

where

$$z_i = (r_1 x_i + r_2)[1 - \sin^2(\theta - \beta) \sin^2 \chi_1]^{-1/2}.$$

As a bonus, this analysis also produces the absorption correction for a cylindrical sheath (window), sur-

rounding a crystal of conventional size, such as may be encountered in low-temperature studies. It is given by:

$$I/I_0^0 = \exp[-\mu(\varrho_2 - \varrho_1 + \sigma_2 - \sigma_1)] \\ = \exp(-\mu(R_2 - R_1)\{[1 - \sin^2(\theta - \beta) \sin^2 \chi_1]^{-1/2} \\ + [1 - \sin^2(\theta + \beta) \sin^2 \chi_1]^{-1/2}\}) \quad (4)$$

where, in this case, the subscripts 1 and 2 respectively, apply to inner and outer radii.

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An X-ray Diffraction Investigation of Liquid Mercury

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X-ray diffraction intensities of liquid mercury have been measured at room temperature with Mo $K\alpha$ radiation. Balanced filters in the diffracted beam and a scintillation counter were used for monochromatization. The structure factor agrees well with published data of Halder & Wagner though the experimental procedures differ considerably. The calculated resistivity ($90 \mu\Omega\text{.cm}$) agrees with the experimental value ($94 \mu\Omega\text{.cm}$). The first peak in the reduced radial distribution function is higher and narrower than for other melts indicating that the difference between the structures of liquid mercury and the other melts is probably not due to the presence in liquid mercury of several structures with different nearest neighbour distances.

Introduction

The structure factor $i(k)$ is calculated from the coherent part of the X-ray scattering where $k = 4\pi \sin \theta / \lambda$, 2θ is the angle between the primary beam and the diffracted beam and λ is the wavelength of the radiation used. By Fourier transformation of $k \cdot i(k)$ the term $r \cdot g(r)$ is obtained. $[g(r) + \varrho_0] / \varrho_0$ is the probability of finding an atom at distance r if there is an atom at the origin, and it is normalized to unit probability at large r . ϱ_0 is the average atomic density of the liquid.

A number of diffraction investigations were carried out on liquid mercury. Recent results obtained at room temperature are summarized in Table 1. Most studies were made with Mo $K\alpha$ radiation using a crystal monochromator. They are marked Mo, CM. The markings,

βF and BF indicate approximate monochromatization with β -filters or balanced filters. The position k_1 of the first peak in $i(k)$ is the quantity resulting most directly from the experiment. The published values agree well with each other with few exceptions. Values in brackets were taken from published curves or calculated from other data. In order to get the height of the first peak $i(k_1)$ it is necessary to scale the measured intensities into absolute units. Experimental errors and errors resulting from the scaling are responsible for the fact that the highest value in the table is 50% higher than the lowest one. The disagreement concerning the height of the first peak $r_1 \cdot g(r_1)$ is even greater. Varying results are reported for the positions and amplitudes of further maxima and minima in real and reciprocal space.

In the present work some systematic errors which