Table 3. *Relationship between x and y for cylinders of unit radius*

x	0	0·000001	0·00001	0·0001	0·001	0·01	0·1	1
y	0	0·003	0·009	0·03	0·1	0·3	0·9	2

6. Applications

6.1. *The geometry of laser fusion*

When apparatus is designed for laser fusion, consideration is given to arranging several pairs of inward-pointing lasers so that the axes of their beams intersect at a point. If the laser beams are assumed to have circular cross sections, the volume illuminated by all the lasers will be the intersection of right circular cylinders. For reasons of thermal stability of the excited plasma at the centre, the lasers are usually arranged in a symmetrical fashion. Here various possible arrangements have been considered.

6.2. *Dissolution of cubic crystals*

The morphologies of partially dissolved crystals are frequently rounded (Heimann, 1975), but edges and vertices may still be well defined. A dissolution shape depends on the starting conditions and continuously changes as dissolution proceeds (Frank, 1972). Even if the chamfering of edges may be approximated by parts of cylindrical surfaces, which eventually join with others from parallel edges to form completed cylinders, it would be unusual for a dissolving crystal if the axes of such cylinders passed through a single point. The edges grouped around a given symmetry axis of a dissolved crystal often fail to meet on the axis as they should in an ideally symmetric body; and in etching experiments surface roughening and etch pitting often mask any underlying ideal morphology. Notwithstanding these misgivings, there are rare occasions when some of the solids depicted here resemble actual dissolution bodies. For example, Fig. 2 bears a similarity to dissolved crystals of the diamond structure [Ellis, 1954; Batterman, 1957 (see Fig. 11, p. 1239); Moore & Lang, 1974].

7. Concluding remarks

All the regular and quasi-regular solids for intersecting cylinders have been drawn, we believe for the first time. They may have relevance in certain applications, but in any case they have a beauty of their own.

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References

ARCHIMEDES (*ca.* 250 BC). *The Method.* English translation by T. L. HEATH (1912). Reprinted 1953. New York: Dover.
BATTERMAN, B. W. (1957). *J. Appl. Phys.* **28**, 1236-1241.
DAVENPORT, H. (1968). *The Higher Arithmetic*, p. 126. London: Hutchinson.
ELLIS, R. C. (1954). *J. Appl. Phys.* **25**, 1497-1499.
FEJES TÓTH, L. (1964). *Regular Figures*, ch. IV. Oxford: Pergamon.
FRANK, F. C. (1972). *Z. Phys. Chem.* (*Frankfurt am Main*), **77**, 84-92.
GARDNER, M. (1962). *Sci. Am.* **207**(5), 164.
HEIMANN, R. B. (1975). *Auflösung von Kristallen.* Vienna: Springer.
HUBBELL, J. H. (1965). *J. Res. Natl Bur. Stand. Sect. C*, **69**(2), 139-143.
MOORE, M. (1973). PhD thesis, Univ. of Bristol, Vol. 1, p. 17.
MOORE, M. (1974). *Math. Gaz.* **58**, 181-185.
MOORE, M. & LANG, A. R. (1974). *J. Cryst. Growth*, **26**, 133-139.
ROBERTSON, S. A. & CARTER, S. (1970). *J. London Math. Soc.* (2), **2**, 125-132.

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Treatment of Enhanced Zones and Rows in Normalizing Intensities

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Abstract

Contrary to the recommendation in some textbooks, enhanced reflexions should not be divided by the enhancement factor in forming general averages for normalization. The intensity required for the enhancement is drawn from the adjacent reflexions in the reciprocal lattice, and the correct average intensity is obtained by including all reflexions at their observed intensity. Weights based on the *number* of reflexions of different types intercepted by the spherical shell that defines those included in the average may be appropriate.

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Introduction

Symmetry elements can be divided into two types: those that cause systematic absences and those that do not. Those producing systematic absences (glide planes, screw axes) produce at the same time groups of reflexions (confined to zones or rows in reciprocal space, respectively) with an average intensity an integral multiple of the general average. As in the case of lattice centring, the fraction of reflexions missing and the integer multiplying the average are related in such a way that the overall average intensity is unchanged. The mechanism for compensation for the reflexions with enhanced intensity is obvious. Certain symmetry elements not producing absences (mirror planes and rotation axes) cause equivalent atoms to coincide in a plane or a line projection, and hence produce a zone or row in reciprocal space for which the average intensity is an integral multiple of the general average (Wilson, 1950). Further alterations of the intensity distribution occur if two or more such symmetry elements are present in the space group. Such multiple enhancements were treated in detail by Rogers (1950). There is, however, no obvious mechanism for compensation for this enhancement. When reflexions are few compensation, or lack of it, may be an important matter in assigning an approximate absolute scale by comparing observed and calculated intensities.

Wilson and Nigam (Wilson, 1964; Nigam, 1972; Nigam & Wilson, 1980), noting that in such cases the finite size of atoms results in forbidden ranges of positional parameters, have shown that there is a general diminution of the intensity of layers (rows) in the immediate neighbourhood of the enhanced zones (rows), just sufficient to compensate for the enhancement. In forming general averages, therefore, reflexions from enhanced zones or rows should be included at their full intensity, not divided by the multiplier, though the latter procedure is recommended in many textbooks of crystallography. One could argue for the former procedure on general grounds of conservation of energy. Within the approximation of the dynamical theory of X-ray diffraction, each atom scatters a definite quantity of energy from the incident beam, and interference, constructive or destructive, merely determines where the energy is located in reciprocal space, without altering the total amount. If any reflexions are included at reduced weight in general averages, the general averages will tend to be lower than the theoretical value

$$\Sigma = \sum_{j=1}^{N} |f_j|^2, \tag{1}$$

and a bias will result. A detailed calculation in a particular case, however, may be more convincing.

The effect of a mirror plane

In the case of a mirror plane perpendicular to c, the $hk0$ reflexions are doubled in average intensity, and the average intensity in the rest of reciprocal space is modulated by the single-slit diffraction function $(\sin x)/x$. The expression for the average intensity, as a function of l, is

$$\langle I \rangle = (1+k)\Sigma \tag{2}$$

where

$$k = 1, \quad l = 0, \tag{3}$$

$$= -(\sin \beta l)/(\pi - \beta)l, \quad |l| > 0. \tag{4}$$

$\beta = 4\pi a/c$ and a is an average atomic radius (Wilson, 1964). The value of K, the sum of k over all l, is

$$K = 1 - 2\sum_{l=1}^{\infty} (\sin \beta l)/(\pi - \beta)l. \tag{5}$$

The series in (5) is well known and sums to unity, so that

$$K = 0. \tag{6}$$

The average intensity, with the $hk0$ reflexions included at their full value, is thus correct.

The preceding calculation was based on the entire reciprocal lattice. The practical procedure is to average the reflexions included within a spherical shell in reciprocal space, and the upper limit of l is not ∞ but some finite value, L. By a fortunate geometrical coincidence, the area of a constant-l plane intercepted between the two spheres determining the shell is independent of l for values of $l < L$, and thus the number of reflexions included for each value of $l < L$ is constant except for edge effects. The average intensity of the reflexions included within the shell is then

$$\langle I \rangle = (1 + \langle K \rangle)\Sigma, \tag{7}$$

where

$$\langle K \rangle = (2L+1)^{-1}[1 - 2\sum_{l=1}^{L} (\sin \beta l)/(\pi - \beta)l] \tag{8}$$

$$= 2(2L+1)^{-1} \sum_{L+1}^{\infty} (\sin \beta l)/(\pi - \beta)l. \tag{9}$$

The series consists of terms of varying sign and magnitude decreasing as l^{-1}. By various approximations [such as replacing it by a sine integral (Abramowitz & Stegun, 1970, ch. 5)], the series can be shown to be of the order of $(2L+1)^{-1}$, so that $\langle I \rangle$, with $hk0$'s included at full weight, departs from its ideal value Σ by a fraction of the order of $(2L+1)^{-2}$. On the other hand, if the $hk0$'s are included only at half weight, the initial 1 in the brackets in (8) is replaced by $\frac{1}{2}$, cancellation is less complete, and $\langle I \rangle$ differs from its ideal value by a fraction of the order of $(2L+1)^{-1}$. Whether either fraction is non-negligible depends on the value of L and the purpose for

which the average is required, but it is (i) less work and (ii) more nearly exact, *not* to weight the *hk*0 reflexions.

Other symmetry elements

A rotation axis of order n parallel to c gives 00l reflexions of n-fold intensity, while the average intensity in the rest of reciprocal space is modulated by the diffraction function $J_1(x)/x$ (Nigam & Wilson, 1980*). The enhanced intensity of the 00l reflexions is compensated if the entire reciprocal lattice is considered, but (unlike the areas of the constant-l planes considered above) the lengths of constant-*hk* rows intercepted by a concentric shell are not independent of *hk*, and it may be worth while to allow for the differences in intercepted length in forming averages.

There is a somewhat similar phenomenon associated with a centre of symmetry; though there are no enhanced reflexions, the average intensity in reciprocal space is modulated by a spherical Bessel function (Wilson, 1981); this effect is likely to be small compared with the larger stereochemical effects discussed there.

* In this paper there is confusion about the meaning of the symbol s. It is not $(2\sin\theta)/\lambda$ as is stated in the *Abstract*, but the projection of this quantity on to a plane perpendicular to the cylinder axis - this is clear from the introduction of the symbol in the context of their equation (4). Nigam & Wilson considered, in fact, only twofold axes, but their equations are valid also for the axes 3, 4 or 6 if the average atomic radius a is replaced by $\sqrt{3}a/2$, $\sqrt{2}a$ or $2a$ respectively.

References

ABRAMOWITZ, M. & STEGUN, I. A. (1970). *Handbook of Mathematical Functions.* New York: Dover.
NIGAM, G. D. (1972). *Indian J. Pure Appl. Phys.* **10**, 655-656.
NIGAM, G. D. & WILSON, A. J. C. (1980). *Acta Cryst.* A**36**, 832-833.
ROGERS, D. (1950). *Acta Cryst.* **3**, 455-464.
WILSON, A. J. C. (1950). *Acta Cryst.* **3**, 258-261.
WILSON, A. J. C. (1964). *Acta Cryst.* **17**, 1591-1592.
WILSON, A. J. C. (1981). *Acta Cryst.* A**37**, 808-810.

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On the Real Part of the Anomalous-Dispersion Term of Atomic Scattering Factors. I. Experimental Part

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Abstract

The wavelength dependence of Si structure factors was measured by the *Pendellösung* method described in the paper of Saka & Kato [*Acta Cryst.* (1986). A**42**, 469-478] in the range from 0·8 down to 0·3 Å with an accuracy level better than 0·05% in most cases. The same conclusion as Takeda & Kato [*Acta Cryst.* (1978). A**34**, 43-47] was obtained; namely that Cromer & Liberman's theory of anomalous dispersion [Cromer & Liberman (1970). *J. Chem. Phys.* **53**, 1891-1898] is essentially correct. As a consequence Jensen's magnetic-scattering term [Jensen (1979). *Phys. Lett.* A, **74**, 41-44] is not acceptable.

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1. Introduction

In some diffraction problems an accurate value for the scattering amplitude depends on the anomalous dispersion. Examples are accurate determination of the charge density through the measurement of the crystal structure factor (F_g) and phase determination by the use of synchrotron radiation or any X-ray source having a continuous spectrum.

The fundamental theory of anomalous dispersion has been well established. Historically important literature can be seen in the textbook of James (1982) and the symposium report edited by Ramaseshan & Abrahams (1975). The relativistic treatment of this problem is described in the standard textbooks on quantum electrodynamics (Heitler, 1954; Akhiezer & Beresteskii, 1965). The theory was developed by

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