und die beiden Zahlen voneinander verschieden, so stellen s_n und s_m auf keinen Fall gleiche Symmetrie-Operationen dar. Andernfalls erhält man durch Gleichsetzen entsprechender Matrixelemente bzw. Vektorkomponenten ein System von linearen Gleichungen über den Unbekannten. Falls es gelingt, das Gleichungssystem zu lösen, so kann man s_n und s_m zu einer Symmetrie-Operation $\{R|v\}$ vereinigen. Wenn die Menge der in dieser Weise gewonnenen Symmetrie-Operationen eine vollständige Gruppe bildet, so ist sie die gesuchte Superraumgruppe. Allgemein ist sie jedoch nicht die einzige Lösung. Andere mögliche Superraumgruppen erhält man dadurch, daß man den Nullpunkt des zweiten Teilsystems relativ zu demjenigen des ersten verschiebt.

Verlegt man den Nullpunkt auf den Endpunkt eines Vektors **u**, so wird die Symmetrie-Operation $\{\mathbf{R}|\mathbf{v}\}$ zu $\{\mathbf{R}|\mathbf{v}+\mathbf{Ru}-\mathbf{u}\}$ transformiert. Wenn zum Beispiel die Raumgruppen beider Teilsysteme *Fmm*2 sind, so kann **u** die Werte (0, 0, 0), (1/4, 0, 0), (0, 1/4, 0) oder (1/4, 1/4, 0) einnehmen. Aus jedem **u** ergibt sich eine andere Superraumgruppe. Allgemein stellt man **u** mit unbekannten Komponenten wie (u, v, w) oder $(u, v, 0)$ dar und bezieht es gleich in die Rechnung ein. Die möglichen Werte der Unbekannten werden nach dem eben beschriebenen Verfahren bestimmt. Wenn wir die Auslöschungsgesetze jeder einzelnen möglichen Superraumgruppe mit den beobachteten Auslöschungen vergleichen, können wir die Superraumgruppe im besten Fall eindeutig bestimmen. Hierzu ist allerdings notwendig, die eigentlichen Satellitenreflexe zu beobachten.

Die hier beschriebene Methode sowie das Verfahren zur Herleitung der Auslöschungsgesetze wurden in *COMMON LISP* (Yuasa & Hagiya, 1985) programmiert und in ein Programmsystem* eingebaut. Die Einzelheiten der Methode sind dem Quelltext des Programms zu entnehmen, dessen neueste Version direkt bei den Verfassern erhältlich ist. Das Programmsystem schließt noch Programme ein, die die Einschränkungen der Parameter von Atomen in speziellen Lagen ermitteln.

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An alternative approach to helical diffraction.

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Abstract

It is shown that by considering the cylindrically averaged intensity diffracted by a non-crystalline fiber as being due to the atoms in one *c* repeat, rather than, as is usual, one helix repeat, some relationships in fiber diffraction can be easily derived. These include the helix selection rule, a new expression for the diffracted intensity, and the cylindrically averaged Patterson. This approach may have other applications as well.

The intensity $I_l(R)$ diffracted by a non-crystalline fiber is equal to the cylindrically averaged intensity of the Fourier transform of a single molecule (Franklin & Klug, 1955; Klug, Crick & Wyckoff, 1958; Millane, 1988) and is given by

$$I_l(R) = \sum_{n\in\mathcal{S}} |G_{nl}(R)|^2 \tag{1}$$

where the Fourier-Bessel structure factors are given by

$$G_{nl}(R) = \sum_{j\in\mathcal{H}} f_j J_n(2\pi R r_j) \exp\left[i(-n\varphi_j + 2\pi l z_j/c)\right]. \tag{2}$$

In these equations, (R, ψ, Z) denotes a cylindrical polar coordinate system in reciprocal space, l indexes the layer lines, (r_j, φ_j, z_j) are the cylindrical coordinates of the jth atom that has scattering factor f_j, c the molecular repeat distance and $J_n(x)$ is the nth-order Bessel function of the first kind. $\mathcal{S}$ denotes the set of integers n that satisfy the helix selection rule (Cochran, Crick & Vand, 1952)

$$l = um + vn \tag{3}$$

where m is any integer, the molecule has u_v helix symmetry (*i.e.* there are u helix repeat units in v turns) and $\mathcal{H}$ is a set of integers that index the atoms in one helix repeat.

The helix selection rule is generally derived by considering the transform of a discontinuous helix as being the convolution of the transform of a continuous helix with that of a set of planes to determine which Bessel orders contribute on each layer line (Cochran, Crick & Vand, 1952; Sherwood, 1976). However, the selection rule can be derived formally and straightforwardly by considering diffraction by the whole c repeat as follows. In the absence

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of any helix symmetry, the diffracted intensity is given by

$$I_l(R) = \sum_{n\in\mathcal{I}} |G'_{nl}(R)|^2 \tag{4}$$

and

$$G'_{nl}(R) = \sum_{j\in\mathcal{C}} f_j J_n(2\pi R r_j) \exp[i(-n\varphi_j + 2\pi l z_j/c)] \tag{5}$$

where $\mathcal{I}$ denotes the set of all integers and $\mathcal{C}$ denotes all the atoms in one c repeat. In the presence of u_v helix symmetry, an atom with coordinates (r, φ, z) in one helix repeat unit is accompanied by an atom in each of $u-1$ consecutive helix repeats that has coordinates $(r, \varphi + 2\pi pv/u, z + pc/u)$, where $p = 1, 2, \ldots, u-1$. Hence, (5) may be rewritten as

$$G'_{nl}(R) = \sum_{p=0}^{u-1} \sum_{j\in\mathcal{H}} f_j J_n(2\pi R r_j) \exp\{i[-n(\varphi_j + 2\pi pv/u) + 2\pi l(z_j/c + p/u)]\} \tag{6}$$

and use of (2) shows that

$$G'_{nl}(R) = G_{nl}(R) \sum_{p=0}^{u-1} \exp[i2\pi p(l-nv)/u]. \tag{7}$$

The sum in (7) is non-zero only if $(l-nv)$ is a multiple of u, *i.e.*

$$l - nv = mu, \tag{8}$$

which is the selection rule (3). So, (4) and (5) then reduce to (1)-(3). The computational significance is that for high helix symmetry (large u) there is a substantial advantage, by a factor of approximately $u^2/2$, in using (1) and (2) rather than (4) and (5).

The expressions (4) and (5) can be used to derive an informative expression for the intensity. Substituting (5) into (4) gives

$$I_l(R) = \sum_{j\in\mathcal{C}} \sum_{k\in\mathcal{C}} f_j f_k \exp[i2\pi l(z_j - z_k)/c] \times \sum_{n\in\mathcal{I}} J_n(2\pi R r_j) J_n(2\pi R r_k) \times \exp[-in(\varphi_j - \varphi_k)] \tag{9}$$

and the summation over n can be evaluated using the addition theorem for Bessel functions (Abramowitz & Stegun, 1972, equation 9.1.79) giving

$$I_l(R) = \sum_{j\in\mathcal{C}} \sum_{k\in\mathcal{C}} f_j f_k J_0(2\pi R r_{jk}) \exp[i2\pi l(z_j - z_k)/c], \tag{10}$$

where r_{jk} is the distance between atoms j and k projected onto a plane normal to the z axis. This can only be derived by ignoring the helix symmetry since the addition theorem requires summation over all Bessel orders.

Equation (10) is a generalized version of a formula derived by Worthington & Elliott (1989) for a helical structure containing a single atom in the helix repeat (*i.e.* a helical lattice) as is now shown. For a helix repeat containing a single, unit amplitude, point atom at radius r_0, (10) becomes

$$I_l(R) = \sum_{j=l}^{u} \sum_{k=1}^{u} J_0(2\pi R r_{jk}) \exp[i2\pi l(z_j - z_k)/c] \tag{11}$$

where

$$r_{jk} = 2r_0 \sin|\pi v(j-k)/u| \tag{12}$$

and

$$z_j - z_k = (j-k)c/u. \tag{13}$$

Substitution of (12) and (13) into (11) allows it to be contracted to

$$I_l(R) = u + 2\sum_{j=1}^{u-1} (u-j) J_0(2\pi R \Delta r_j) \cos(2\pi lj/u), \tag{14}$$

where $\Delta r_j = r_{j+k,k}$, and rearrangement of the terms in the summation gives

$$I_l(R) = u \sum_{j=1}^{u} J_0(2\pi R \Delta r_j) \cos(2\pi lj/u) \tag{15}$$

which is identical to equation (21) of Worthington & Elliott (1989). This simplification only comes about when there is one atom in the helix repeat so that (12) and (13) apply.

Equation (10) can also be used to show that the function $Q(r, z)$ defined by

$$Q(r, z) = \sum_{l=-\infty}^{\infty} \int_0^{\infty} I_l(R) J_0(2\pi R r) \exp(i2\pi l z/c) R \, \mathrm{d}R \tag{16}$$

(MacGillavry & Bruins, 1948) is the cylindrically averaged Patterson of the structure. For point atoms with atomic numbers Z_j, substitution of (10) into (16) and use of the orthogonality of the Bessel and trigonometric functions gives

$$Q(r, z) = (c/4\pi^2 r) \sum_{j\in\mathcal{C}} \sum_{k\in\mathcal{C}} Z_j Z_k \delta(r - r_{jk}) \delta(z - z_j + z_k), \tag{17}$$

where $\delta(x)$ is the Dirac delta function, which shows that $Q(r, z)$ is, indeed, the cylindrically averaged Patterson. Note that the sum in (17) should include the interatomic vector components $(z_j - z_k)$ between different c repeats. This analysis also emphasizes that the cylindrically averaged Patterson is independent of the helix symmetry.

In summary, some relationships in fiber diffraction can be straightforwardly derived by using the helix-symmetry-independent form of the diffracted intensity given by (4) and (5). This approach may also be useful in other applications. Equation (10), which does not appear to have been derived previously, may also be useful.

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In order to facilitate the handling of requests for IUCr sponsorship and support of scientific meetings, the Executive Committee has decided that requests must reach the Chairman of the IUCr Calendar Sub-committee no later than nine months before the start of the meeting. The change will allow proper publicity of the sponsorship in the literature to be distributed, and earlier funding of conferences. The change (from a six month deadline) will go into effect three months after the first appearance of this notice. The present Chairman of the IUCr Calendar Sub-committee is Professor P. Coppens, Department of Chemistry, State University of New York at Buffalo, Acheson Hall, Buffalo, NY 14214, USA, from whom the sponsorship request forms may be obtained.

Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Acta Cryst. (1991). A**47**, 451

Crystal engineering: the design of organic solids. By G. R. DESIRAJU. Pp. xiv+312. Amsterdam and New York: Elsevier Scientific Publishers, 1989. Price Dfl 220.00 or US $115.75. A review of this book, by Stephen J. Maginn, has been published in the June 1991 issue of *Journal of Applied Crystallography*, page 265.

A guide to materials characterisation and chemical analysis. By JOHN P. SIBILIA. Pp. x+318. Weinheim: VCH Verlagsgesellschaft, 1988. Price DM 75.00, £25.95. A review of this book, by David F. Rendle, has been published in the June 1991 issue of *Journal of Applied Crystallography*, pages 265-266.

Monteregian treasures. By J. A. MANDARINO and V. ANDERSON. Pp. xiii+281. Cambridge University Press, 1989. Price £60.00, US $85.00. ISBN 052132632X. A review of this book, by James E. Chisholm, has been published in the June 1991 issue of *Journal of Applied Crystallography*, page 266.