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Short Communications

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Acta Cryst. (1959). **12**, 71

Calculation of scattering intensity from a cylindrically symmetrical system.

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G. Oster & D. P. Riley (1952) give an expression for the amplitude of scattering F in the equatorial plane by a cylindrically symmetrical system

$$F = \frac{\int_0^\infty rG(r)J_0(kr)\,dr}{\int_0^\infty rG(r)\,dr}\,.$$

Here F is normalised to be unity at zero scattering angle and $k = (4\pi/\lambda)\sin\theta$ where λ is the wavelength of the incident radiation and 2θ is the scattering angle. $G(r)da$ is the probability that scattering material lies in the element of area da at distance r from the centre of the equatorial section.

When
$$\begin{aligned} G(r) &= \cos^2\frac{m\pi r}{R} & r &< R \\ &= 0 & r &\geq R \end{aligned}$$

the structure is said to be radially periodic. In this case $2m$ is the number of 'corrugations' in the distribution of scattering material across a diameter $2R$ of the equatorial section. If we define a new parameter $p = kR/(2m\pi)$, we can write

$$F(p) = \frac{\int_0^{2m\pi} x(1+\cos x)J_0(px)\,dx}{\int_0^{2m\pi} x(1+\cos x)\,dx}\,.$$

We discuss the evaluation of F when $2m$ is an odd integer, which is the case when there is a whole number of corrugations across a diameter. Oster & Riley (1952) state that F can be reduced to 'a complicated algebraic expression involving k, $2m\pi/R$, $J_0(kR)$, $J_1(kR)$', and from this expression appear to have inferred a maximum of F^2 at $p = 1$. The author has been unable to find such an expression; and to calculate F for $0 < p < \infty$ three series expansions have been derived, each suitable for calculation on a limited range. Further it can be shown that a maximum of F^2 occurs near, but not at, $p = 1$. For $2m = 7$ this maximum is at $p = 1{\cdot}038$, and the value there of F^2 exceeds that at $p = 1$ by 38%.

We list these three series below, giving a rough guide to their appropriate ranges and the number of terms needed to obtain $\sim 1\%$ accuracy.

A. A series expansion of $F(p)$, centred on $p = 1$ and convergent for all values of p. For 1% accuracy no more than 10 terms are needed in the range $1-1/(2m) < p < 1+1/(2m)$

$$F = 2\left[1-\frac{1}{(m\pi)^2}\right]^{-1}\sum_{n=0}^{n=\infty}\frac{[m\pi(1-p^2)]^n}{n!}\cdot\frac{J_{n+2}(2m\pi)}{2n+3}\,.$$

B. A series expansion of $F(p)$, centred on $p = 0$ and convergent for $p < 1$. For 1% accuracy we can neglect terms of order p and higher, in the range $0 < p < 1/(2m)$.

$$F = \frac{2}{1-p^2}\left[1-\frac{1}{(m\pi)^2}\right]^{-1}$$
$$\times\left\{\frac{J_1(2m\pi p)}{2m\pi p}-\frac{1}{(2m\pi)^2}\left[1+J_0(2m\pi p)\right.\right.$$
$$+\left(\frac{p}{2}\right)^2\{2(1+J_0(2m\pi p))-2J_2(2m\pi p)\}\ldots$$
$$+\left(\frac{p}{2}\right)^n\{{}^{2n}C_n(1+J_0(2m\pi p))-2\,{}^{2n}C_{n-1}J_2(2m\pi p)\ldots$$
$$\left.\left.+(-)^nJ_{2n}(2m\pi p)\}\right]\right\}$$

C. An expansion asymptotic to F for large values of $p(1-p^2)$.

We give the leading terms of this expansion, these being sufficient to calculate F to $\sim 1\%$ accuracy in the ranges $1/(2m) < p < 1-1/(2m)$; $1+1/(2m) < p < \infty$

$$F = \frac{2}{1-p^2}\left[1-\frac{1}{(m\pi)^2}\right]^{-1}\left\{\frac{J_1(2m\pi p)}{2m\pi p}-\frac{1}{(2m\pi)^2}\left[\begin{matrix}0,\ p>1;\\(1-p^2)^{-\frac{1}{2}},\ p<1\end{matrix}\right]\right.$$
$$\left.-\frac{1}{(2m\pi)^2}\cdot\frac{(2m\pi p)^{-\frac{1}{2}}}{1-p^2}\cdot\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\left(\begin{matrix}\cos\left(2m\pi p-\frac{\pi}{4}\right)\cdot\left[1-\frac{9+30p^2+345p^4}{2![16m\pi p(1-p^2)]^2}+\ldots\right]\\+\sin\left(2m\pi p-\frac{\pi}{4}\right)\cdot\left[\frac{1-9p^2}{16m\pi p(1-p^2)}-\frac{225-315p^2-17325p^4-28{,}665p^6}{3![16m\pi p(1-p^2)]^3}\right]\end{matrix}\right)\right\}.$$

In an interpretation of the scattering pattern of keratin, R.D.B. Fraser & T. McRae (Private communication) evaluated F^2 for $2m = 7$ and p in the range $0{\cdot}15 < p < 1{\cdot}13$, using the series A and C. The graph of F^2 in this range is shown in Fig. 1.

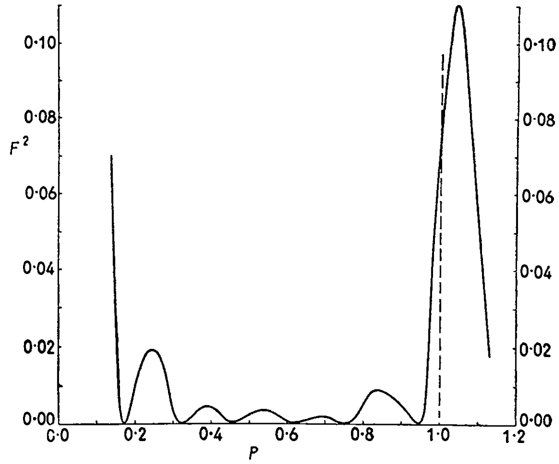

Fig. 1. Plot of scattering intensity against $p = kR/(2m\pi)$ for $2m = 7$.

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The unit-cell dimensions and space group of monoclinic $NiSO_4.6H_2O$.

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Crystals of the green monoclinic hexahydrate of nickel sulphate, which is unstable at room temperature, were obtained by the slow evaporation of a cold mixture of solutions of disodium adenosine triphosphate and nickel sulphate whilst trying to crystallize a heavy atom salt of the nucleotide. The unit-cell dimensions of two different crystals, determined from rotation and Weissenberg photographs, are given in Table 1.

Table 1. *Unit-cell dimensions*

	Crystal 1	Crystal 2
a (Å)	9·84	11·58
b (Å)	7·17	6·09
c (Å)	24·0	23·9
β (°)	97·5	94·0

The axial ratios of crystal 1 (1·372:1:3·347) agree with those quoted by Groth when the c axis of his crystal is doubled (1·3723:1:3·3526, $\beta = 98°\ 15'$). Crystal 1 is also isomorphous with the modification of $MgSO_4.6H_2O$ studied by Ide (1938), ($a = 10{\cdot}04$, $b = 7{\cdot}15$, $c = 22{\cdot}34$ Å, $\beta = 98°\ 34'$, space group given as $C2/c$).

The measured density $2{\cdot}0\pm0{\cdot}1$ g.cm.$^{-3}$ corresponds to the more accurate value 2·036 quoted in Groth; the calculated value for 8 molecules per unit cell is 2·07 for both crystals 1 and 2.

For both crystals reflexions hkl are absent when $h+k$ is odd, but there are no other systematic lattice absences; the space group may thus be either $C2/m$, Cm or $C2$.

For crystal 1, the absence of peaks along the line $z = 0$ in the $0kl$ sharpened Patterson projection precludes a mirror plane perpendicular to b, but the presence of peaks along $y = 0$ indicates a two-fold axis parallel to b; the space group is probably $C2$. Although there is no glide-plane perpendicular to the diad axis, the $00l$ reflexions with l odd are absent, suggesting that the z coordinates of at least the nickel atoms are in accordance with the space group $C2/c$.

No further work on this compound is contemplated.

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