

provided that E is known, V_h and V_{2h} can be calculated from the experimental values of the three ratios.

Fig. 1 gives an experimental result for magnesium oxide. The abscissa is V_{111} and the ordinate, V_{222} . The accelerating voltage is 100 kV. From each experimental value of the ratios, a curve is drawn on the diagram. The values of V_{111} and V_{222} are determined from the intersection of the curves. The error can also be estimated as shown by broken lines in the Figure. The values obtained were $V_{111} = 1.78 \pm 0.05$ and $V_{222} = 3.90 \pm 0.10$ volt. The former value is in good accord with that of Lehmpfuhl (1972).

In many cases, the fringe distance is too large at the second-order position for an accurate value of l_{2h} to be determined. The second method is proposed for such a case. In this method, no fringes at the second order are required, while those at the first-order position and the symmetric position must be taken at least at two different accelerating voltages. Then, V_h and V_{2h} can be calculated from the ratios l_{sym}/l_h at these voltages. No experiment has yet been carried out with this method. A calculation was done to estimate the accelerating voltages adequate for the measurement.

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A note on the higher-moment test for space-group determination. By S. PARTHASARATHY, *Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras-600025, India**

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Theoretical expressions for the second, third and fourth moments of normalized intensity z and the fourth moment of the intensity (I) scattered by an asymmetric unit are given for crystals in which all atoms are in general positions. The expression for the fourth moment of I applicable to crystals containing atoms in both general and different types of special position is also given.

Foster & Hargreaves (1963*b*) have given in Table 1 of their paper the expressions for the first three moments of the intensity (I) scattered by the asymmetric unit and these results are applicable to crystals (containing atoms at general positions in the unit cell) belonging to all but two of the 74 space groups and the nine related plane groups in the triclinic, monoclinic and orthorhombic systems. They have also shown how these results could be used to derive the theoretical expressions for the second and third moments of the normalized intensity (z) when the crystal contains atoms in both general and special positions. In this note we shall list the expressions for the fourth moment of the intensity (I), since in some cases the tests based on the second and third moments of z may not be very effective. For example, for crystals containing a few (*i.e.* one or two) dominating heavy atoms besides a large number of light atoms, it may be useful to employ the fourth moment of z . This is clear from Table 1 (computed from the results of Parthasarathy, 1966) which lists the higher moments of z for crystals containing one or two dominating atoms besides a large number of light atoms (for brevity referred to as the one-atom case and two-atom case respectively) in the space groups $P1$ and $P\bar{1}$ in terms of the parameter σ_1^2 (which is the fractional contribution to the local mean intensity from the heavy atoms in the unit cell.)

Fig. 2 shows a result obtained by assuming the values of l_{sym}/l_{200} at 100, 1000 and 2000 kV. The three curves intersect at approximately 60° . This means that a high-accuracy measurement will be possible if the measurement is done at a conventional voltage around 100 kV and at least at an extremely high voltage over 1000 kV.

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Table 1. Higher moments of z for the one-atom and two-atom cases when the heavy-atom contributions are 0.7, 0.8 and 0.9

The tabulated values have been calculated from the results of Parthasarathy (1966). Note the inefficiency of $\langle z^2 \rangle$ and the distinction of $\langle z^4 \rangle$ in all the cases.

σ_1^2	Space group	One-atom case			Two-atom case		
		$\langle z^2 \rangle$	$\langle z^3 \rangle$	$\langle z^4 \rangle$	$\langle z^2 \rangle$	$\langle z^3 \rangle$	$\langle z^4 \rangle$
0.7	$P1$	1.51	2.96	7.07	1.76	4.14	11.94
	$P\bar{1}$	2.02	5.79	21.17	2.27	7.40	30.93
0.8	$P1$	1.36	2.29	4.55	1.68	3.63	9.31
	$P\bar{1}$	1.72	3.99	11.51	2.04	5.72	19.89
0.9	$P1$	1.19	1.63	2.50	1.60	3.08	6.75
	$P\bar{1}$	1.38	2.37	4.79	1.79	4.07	10.92

Another purpose of this note is to list the *explicit expressions* for the second, third and fourth moments of the normalized intensity z applicable for crystals containing all atoms at general positions in the unit cell, since such crystals are of frequent occurrence. As the expressions for $\langle I^4 \rangle$ for crystals containing atoms in both general and special positions and for $\langle z^n \rangle$, $n=2, 3$ and 4, for crystals containing all atoms in general positions could be derived from the theoretical results of Foster & Hargreaves (1963*a*) we shall give only the final results, omitting all the intermediate steps. The notation followed in this paper is the same as that used by Foster & Hargreaves (1963*a, b*).

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Table 2. Theoretical expressions for the second, third and fourth moments of z and the fourth moment of I for crystals with all atoms in general positions

For the notation see Foster & Hargreaves (1963a, b). The quantities $C(4)$, $C(6)$ and $C(8)$ are characteristic of the given crystal, being determined by the number and the scattering powers of the atoms in the asymmetric unit, and are defined to be $C(2n) = S(2n)/S^n(2)$.

No.	Geometrical structure factor		Expressions for $\langle I^4 \rangle$ and $\langle z^n \rangle$, $n=2, 3$ and 4
1	$A = \cos \theta$ $A = \sin \theta$	$B = \sin \theta$ $B = \cos \theta$	$\langle I^4 \rangle = 24S^4(2) - 72S(4)S^2(2) + 64S(6)S(2) - 33S(8) + 18S^2(4)$ $\langle z^2 \rangle = 2 - C(4)$ $\langle z^3 \rangle = 6 - 9C(4) + 4C(6)$ $\langle z^4 \rangle = 24 - 72C(4) + 64C(6) - 33C(8) + 18C^2(4)$
2	$A = \cos \theta$ $A = \sin \theta$	$B = 0$ $B = 0$	$\langle I^4 \rangle = \frac{105}{16}S^4(2) - \frac{315}{16}S(4)S^2(2) + \frac{35}{2}S(6)S(2) - \frac{1155}{128}S(8) + \frac{315}{64}S^2(4)$ $\langle z^2 \rangle = 3 - \frac{3}{4}C(4)$ $\langle z^3 \rangle = 15 - \frac{45}{2}C(4) + 10C(6)$ $\langle z^4 \rangle = 105 - 315C(4) + 280C(6) - \frac{1155}{8}C(8) + \frac{315}{4}C^2(4)$
3	$A = \cos \theta \cos \phi$ $A = \cos \theta \sin \phi$ $A = \cos \theta \sin \phi$ $A = \sin \theta \sin \phi$	$B = \cos \theta \sin \phi$ $B = \cos \theta \cos \phi$ $B = \sin \theta \sin \phi$ $B = \sin \theta \cos \phi$	$\langle I^4 \rangle = \frac{3}{2}S^4(2) - \frac{9}{2}S(4)S^2(2) + S(6)S(2) - \frac{33}{128}S(8) + \frac{9}{32}S^2(4)$ $\langle z^2 \rangle = 2 - \frac{1}{2}C(4)$ $\langle z^3 \rangle = 6 - \frac{9}{2}C(4) + C(6)$ $\langle z^4 \rangle = 24 - 36C(4) + 16C(6) - \frac{33}{8}C(8) + \frac{9}{2}C^2(4)$
4	$A = \cos \theta \cos \phi$ $A = \cos \theta \sin \phi$ $A = \sin \theta \sin \phi$	$B = 0$ $B = 0$ $B = 0$	$\langle I^4 \rangle = \frac{105}{16}S^4(2) - \frac{315}{16}S(4)S^2(2) + \frac{35}{2}S(6)S(2) - \frac{1155}{1024}S(8)$ $+ \frac{315}{4096}S^2(4)$ $\langle z^2 \rangle = 3 - \frac{3}{4}C(4)$ $\langle z^3 \rangle = 15 - \frac{45}{2}C(4) + \frac{5}{2}C(6)$ $\langle z^4 \rangle = 105 - \frac{315}{2}C(4) + 70C(6) - \frac{1155}{64}C(8) + \frac{315}{16}C^2(4)$
5	$A = \cos \theta \cos \phi \cos \psi$ $A = \cos \theta \sin \phi \sin \psi$	$B = \sin \theta \sin \phi \sin \psi$ $B = \sin \theta \cos \phi \cos \psi$	$\langle I^4 \rangle = \frac{3}{32}S^4(2) - \frac{9}{128}S(4)S^2(2) + \frac{1}{64}S(6)S(2) - \frac{1177}{16384}S(8) + \frac{27}{2048}S^2(4)$ $\langle z^2 \rangle = 2 - \frac{1}{4}C(4)$ $\langle z^3 \rangle = 6 - \frac{9}{4}C(4) + \frac{1}{4}C(6)$ $\langle z^4 \rangle = 24 - 18C(4) + 4C(6) - \frac{1177}{64}C(8) + \frac{27}{8}C^2(4)$
6	$A = \cos \theta \cos \phi \cos \psi$ $A = \cos \theta \sin \phi \sin \psi$ $A = \cos \theta \sin \phi \sin \psi$	$B = \cos \theta \cos \phi \sin \psi$ $B = \cos \theta \sin \phi \cos \psi$ $B = \sin \theta \sin \phi \sin \psi$	$\langle I^4 \rangle = \frac{3}{32}S^4(2) + \frac{9}{128}S(4)S^2(2) - \frac{1}{8}S(6)S(2) + \frac{513}{16384}S(8) + \frac{9}{2048}S^2(4)$ $\langle z^2 \rangle = 2 + \frac{1}{4}C(4)$ $\langle z^3 \rangle = 6 + \frac{9}{4}C(4) - 2C(6)$ $\langle z^4 \rangle = 24 + 18C(4) - 32C(6) + \frac{513}{64}C(8) + \frac{9}{8}C^2(4)$
7	$A = \cos \theta \cos \phi \cos \psi$ $A = \cos \theta \cos \phi \sin \psi$ $A = \cos \theta \sin \phi \sin \psi$ $A = 0$ $A = 0$ $A = 0$	$B = 0$ $B = 0$ $B = 0$ $B = \sin \theta \sin \phi \sin \psi$ $B = \sin \theta \sin \phi \cos \psi$ $B = \sin \theta \cos \phi \cos \psi$	$\langle I^4 \rangle = \frac{105}{4096}S^4(2) + \frac{315}{16384}S(4)S^2(2) - \frac{35}{1024}S(6)S(2) + \frac{1179}{2097152}S(8)$ $+ \frac{315}{262144}S^2(4)$ $\langle z^2 \rangle = 3 + \frac{3}{8}C(4)$ $\langle z^3 \rangle = 15 + \frac{45}{8}C(4) - 5C(6)$ $\langle z^4 \rangle = 105 + \frac{315}{4}C(4) - 140C(6) + \frac{1179}{512}C(8) + \frac{315}{64}C^2(4)$

Table 2 contains the expressions for $\langle z^n \rangle$, $n=2, 3$ and 4 and $\langle I^4 \rangle$ when all atoms are in general positions. The theoretical expression for $\langle I^4 \rangle$ when the atoms are in both general and different types of special position can be shown to be

$$\begin{aligned} \langle I^4 \rangle = & \langle I_g^4 \rangle + \lambda_1^8 \langle I_1^4 \rangle + \lambda_2^8 \langle I_2^4 \rangle + \lambda_3^8 \langle I_3^4 \rangle + K_4 \langle I_g^3 \rangle \{ \lambda_1^3 \langle I_1 \rangle \\ & + \lambda_2^3 \langle I_2 \rangle + \lambda_3^3 \langle I_3 \rangle \} + \langle I_g^2 \rangle [K_5 \{ \lambda_1^4 \langle I_1^2 \rangle + \lambda_2^4 \langle I_2^2 \rangle \\ & + \lambda_3^4 \langle I_3^2 \rangle \} + K_6 \{ \lambda_1^2 \lambda_2^2 \langle I_1 \rangle \langle I_2 \rangle + \lambda_2^2 \lambda_3^2 \langle I_2 \rangle \langle I_3 \rangle \\ & + \lambda_3^2 \lambda_1^2 \langle I_3 \rangle \langle I_1 \rangle \}] + \langle I_g \rangle [K_4 \{ \lambda_1^6 \langle I_1^3 \rangle + \lambda_2^6 \langle I_2^3 \rangle \\ & + \lambda_3^6 \langle I_3^3 \rangle \} + K_6 \{ \lambda_1^4 \lambda_2^2 \langle I_1^2 \rangle \langle I_2 \rangle + \lambda_1^4 \lambda_3^2 \langle I_1^2 \rangle \langle I_3 \rangle \\ & + \lambda_2^4 \lambda_3^2 \langle I_2^2 \rangle \langle I_3 \rangle + \lambda_2^4 \lambda_1^2 \langle I_2^2 \rangle \langle I_1 \rangle + \lambda_3^4 \lambda_1^2 \langle I_3^2 \rangle \langle I_1 \rangle \\ & + \lambda_3^4 \lambda_2^2 \langle I_3^2 \rangle \langle I_2 \rangle \} + K_7 \lambda_1^2 \lambda_2^2 \lambda_3^2 \langle I_1 \rangle \langle I_2 \rangle \langle I_3 \rangle] \\ & + K_5 \{ \lambda_1^4 \lambda_2^4 \langle I_1^2 \rangle \langle I_2^2 \rangle + \lambda_2^4 \lambda_3^4 \langle I_2^2 \rangle \langle I_3^2 \rangle + \lambda_3^4 \lambda_1^4 \langle I_3^2 \rangle \langle I_1^2 \rangle \} \\ & + K_4 \{ \lambda_1^6 \lambda_2^2 \langle I_1^3 \rangle \langle I_2 \rangle + \lambda_1^6 \lambda_3^2 \langle I_1^3 \rangle \langle I_3 \rangle + \lambda_2^6 \lambda_3^2 \langle I_2^3 \rangle \langle I_3 \rangle \} \end{aligned}$$

$$\begin{aligned} & + \lambda_2^6 \lambda_1^2 \langle I_2^3 \rangle \langle I_1 \rangle + \lambda_3^6 \lambda_1^2 \langle I_3^3 \rangle \langle I_1 \rangle + \lambda_3^6 \lambda_2^2 \langle I_3^3 \rangle \langle I_2 \rangle \} \\ & + K_6 \{ \lambda_1^4 \lambda_2^2 \lambda_3^2 \langle I_1^2 \rangle \langle I_2 \rangle \langle I_3 \rangle + \lambda_2^4 \lambda_3^2 \lambda_1^2 \langle I_2^2 \rangle \langle I_3 \rangle \langle I_1 \rangle \\ & + \lambda_3^4 \lambda_1^2 \lambda_2^2 \langle I_3^2 \rangle \langle I_1 \rangle \langle I_2 \rangle \} , \end{aligned}$$

where K_4 , K_5 , K_6 and K_7 are constants having the values 28, 70, 228 and 150 respectively for centrosymmetric plane groups and space groups and the values 16, 36, 96 and 60 respectively for non-centrosymmetric plane groups and space groups.

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