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Note on the intensity distribution in a diffraction maximum.

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In calculations of the intensity distribution in the diffraction maxima from a mosaic crystal, phase differences caused by the divergence of the incident and the convergence of the diffracted beam are usually neglected by assuming that the X-ray source and the detector are at infinite distances from the crystal. For the one-dimensional case of a primitive row of atoms the intensity distribution is then given by the interference function

$$I_i(v) = \sin^2 \pi v / (\pi v)^2$$

in which the intensity $I_i(v)$ is expressed in the height of the main maximum, and the deviation v from the reflection centre in the distance between two successive zeroes (compare, James, 1948, p. 4 and 43).

In practice the experimental conditions are often such that the neglect of the phase differences mentioned above is not justified (Wilson, 1946; Kuznetsov & Terminasov, 1961). Wilson (1946) showed that the additional phase differences ordinarily cause only a negligible broadening of the lines in a Debye–Scherrer pattern. The intensity distribution in the reflections may, however, be affected considerably by the divergence of the incident and diffracted beams.

In order to obtain some idea about this effect, we calculated some intensity distributions $I_f(v)$ for the simple case of the zeroth diffraction maximum from a row of atoms with finite values for the distance between the point source and the 'crystal' (r_1) and the distance between the 'crystal' and the detector (r_2). The line connecting the X-ray source and the centre of the detector was taken perpendicular to the row of atoms and through its centre.

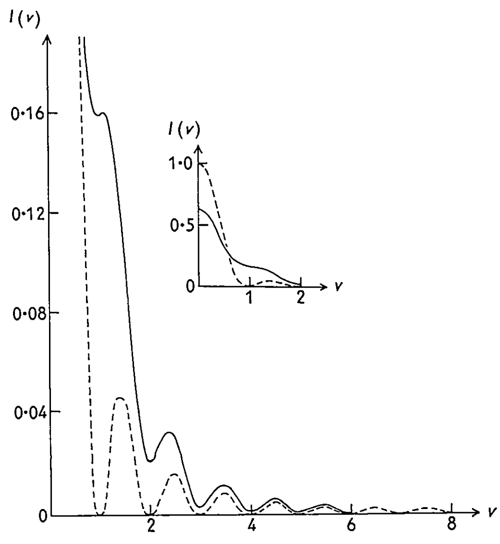

Fig. 1. Comparison of the interference functions $I_i(v)$ (dotted line) and $I_f(v)$ (solid line), the latter calculated for a row of 2001 atoms, $a = 10$ Å, $\lambda = 0{\cdot}7$ Å, $r_1 = 10$ cm., $r_2 = 2{\cdot}5$ cm. The intensities I are expressed in the height of the main maximum of $I_i(v)$, the deviation v from the reflection center in the distance between two successive zeroes in $I_i(v)$.

Fig. 1 shows the results of such a calculation for a row of 2001 atoms, with spacing $a = 10$ Å, $\lambda = 0{\cdot}7$ Å, $r_1 = 10$ cm., $r_2 = 2{\cdot}5$ cm. For this case it appears that the height of the main maximum amounts to only 63% of that of the usual interference function $I_i(v)$. The latter function decreases, however, much more rapidly for increasing distances from the diffraction center than the function $I_f(v)$. At $v = 0{\cdot}60$ the curves intersect, and up to the sixth subsidiary maximum, where the differences become insignificant, $I_f(v)$ remains larger than $I_i(v)$.

Table 1. *Comparison of the integrated intensities* $Q_i(n)$ *and* $Q_f(n)$

n	$Q_i(n)$	$Q_f(n)$	n	$Q_i(n)$	$Q_f(n)$
1	0·90282	0·72072	11	0·99080	0·99064
2	0·94994	0·91560	12	0·99157	0·99144
3	0·96641	0·95707	13	0·99222	0·99212
4	0·97475	0·97109	14	0·99277	0·99269
5	0·97978	0·97798	15	0·99326	0·99319
6	0·98314	0·98212	16	0·99368	0·99362
7	0·98555	0·98491	17	0·99405	0·99400
8	0·98735	0·98693	18	0·99438	0·99434
9	0·98876	0·98846	19	0·99468	0·99464
10	0·98988	0·98966	20	0·99495	0·99491
			∞	1·00000	

For a comparison of the integrated intensities, the surfaces below the curves $I_i(v)$ and $I_f(v)$ were calculated from the $-n$th zero to the $+n$th zero in $I_i(v)$. The corresponding integrated intensities $Q_i(n)$ and $Q_f(n)$ are listed in Table 1; even for $n = 7$ the differences appear to be smaller than 0·1%. The total intensity is thus not affected by the finite values for r_1 and r_2. It may be noted, however, that at the 20th zero, which corresponds with an angular deviation of 2·4′ from the diffraction center for the case considered, the integrated intensities are still 0·5% smaller than the total intensity of the diffraction maximum.

The conclusion that the finite values of r_1 and r_2 which are met in practice do not change the total reflection intensity can easily be extended to the three-dimensions.

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