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Theoretical Corrections for Extinction

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A theoretical extinction correction for structure factors is given.

An approximate theoretical treatment of X-ray diffraction in real crystals has led to a new formula for the integrated intensity (Zachariasen, 1967). The mosaic model of a real crystal is assumed, with approximately spherical perfect crystal domains of radius r and an isotropic Gaussian distribution function $W(\Delta)=\sqrt{2}g\exp(-2\pi g^2\Delta^2)$ for the misorientation. The resulting formula for the observed structure factor, F_o, is in standard notation

$$F_o=F_c[1+2x]^{-1/4}\,,\quad x=r^*K^2Q_0\lambda^{-1}\bar{T}\,,$$

$$r^*=r/[1+(r/\lambda g)^2]^{1/2}\,,\quad \bar{T}=-A^{-1}dA/d\mu_0$$

where $K=1$ for the normal and $K=|\cos 2\theta|$ for the parallel component of polarization. Thus the quantity $[1+2x]^{-1/4}$ represents the theoretical extinction correction for the structure factor.

The formula as given above applies when the absorption is moderately small, but has been modified to include the Borrmann effect for heavily absorbing crystal specimens (Zachariasen, 1968*a*).

Since the extinction effects are dependent upon the single quantity r^*, intensity measurements with two different wave lengths are needed for the experimental determination of both parameters r and g characterizing the real crystal specimen.

The predictions of the theory have been tested experimentally with copper and molybdenum radiation on crystal spheres of quartz and hambergite (Zachariasen, 1968*c*), LiF (Zachariasen, 1968*b*), CaF_2 (Zachariasen, 1968*a*) and phenakite (Zachariasen, 1968*d*). The resulting values of r^*, r and g are:

	$r^*\times10^4$ cm			
	Mo	Cu	$r\times10^4$ cm	$g\times10^{-4}$ rad^{-1}
LiF	0·022	0·045	0·11	0·03
Quartz	0·47	0·46	0·46	>0·7
Phenakite	0·69	1·00	1·2	1·2
Hambergite	0·98	1·54	2·0	1·6
CaF_2	2·5	3·0	3·2	5·7

The agreement between theory and experiment is excellent, and the assumed isotropy as to domain shape and misorientation is satisfactory for these crystal specimens.

References

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DISCUSSION

HAMILTON: We have had some experience using Professor Zachariasen's approximation and have, as he suggested, extended it to a completely general anisotropic treatment. We have considered both type I and type II crystals, the former, which are mosaic spread dominated, involving an anisotropic Gaussian distribution of orientation while the particle shape in the latter is treated as ellipsoidal. We have treated these examples by our least-squares program and in general found a significant improvement in R. It may be worth commenting that the tensors in most cases refine to the correct symmetry even though this restraint is not necessarily inbuilt. Our R factors only come down to 2–3% by contrast with 1–2% of Professor Zachariasen's.

CHANDRASEKHAR: I will just mention that we have tested Professor Zachariasen's formulae using polarized X-rays and have found excellent agreement. (I will discuss this matter in greater detail tomorrow.)