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The Ewald and Darwin solutions for perfect crystals.

By R. J. Weiss, *Materials Research Laboratory, U.S. Army Materials Research Agency, Watertown, Massachusetts, U.S.A.*

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In the course of some measurements of the absolute structure factors of silicon perfect crystals (Bragg case) we found it necessary to consider the criteria for the so called 'thick crystal' case considered by Zachariasen (1945) and Hirsch & Ramachandran (1950). Since the absorption coefficient of silicon for Mo $K\alpha$ is very small we were approaching the cases commonly termed the Ewald and Darwin solutions. In the former the product of the absorption coefficient and crystal thickness is very much less than unity while in the latter case this product is very much greater than unity, the absorption coefficient being very small in both cases. In the common notation of Zachariasen (1945) the Ewald solution gives an integrated intensity $R^y_H=\pi$ as the absorption coefficient approaches zero while the Darwin solution gives $R^y_H=\frac{8}{3}$ in the limit of negligible absorption coefficient. Since the two solutions differ by about 18 % and we were attempting to measure structure factors to 1 % we found it necessary to evaluate the general formula (Zachariasen, 1945, equation 3·139) without the simplifying Darwin assumption employed by Hirsch & Ramachandran (1950) and Zachariasen (1945), equation 3·189.

The integrated intensity in Bragg reflection for a finitely thick plane parallel perfect crystal is given exactly by

$$R^y_H = \int_{-\infty}^{\infty} \frac{P_H}{P_o}\, dy \tag{1}$$

where

$$\frac{P_H}{P_0} = \frac{\sin^2 av + \sinh^2 aw}{\dfrac{|q+z^2|}{|q|} + \left\{\dfrac{|q+z^2|+|z|^2}{|q|}\right\}\sinh^2 aw - \left\{\dfrac{|q+z^2|-|z|^2}{|q|}\right\}\sin^2 av + \frac{1}{2}\left|\left\{\dfrac{|q+z^2|+|z|^2}{|q|}\right\}^2-1\right|^{\frac{1}{2}}\sinh|2aw| + \frac{1}{2}\left|\left\{\dfrac{|q+z^2|-|z|^2}{|q|}\right\}^2-1\right|^{\frac{1}{2}}\sin|2av|} \tag{2}$$

$$av = \frac{A}{\sqrt{2}}\{\sqrt{[(y^2-g^2+k^2-1)^2+4(gy-k)^2]}+(y^2-g^2+k^2-1)\}^{\frac{1}{2}}$$

$$aw = \frac{A}{\sqrt{2}}\{\sqrt{[(y^2-g^2+k^2-1)^2+4(gy-k)^2]}-(y^2-g^2+k^2-1)\}^{\frac{1}{2}} \tag{3}$$

$$\frac{|q+z^2|}{|q|} = \frac{[(y^2-g^2+k^2-1)^2+4(gy-k)^2]^{\frac{1}{2}}}{1+k^2} \tag{4}$$

$$\frac{|z|^2}{|q|} = \frac{y^2+g^2}{1+k^2}\,. \tag{5}$$

Ewald approximation $g\equiv 0$; Darwin approximation $aw\gg 1$.

We have evaluated the case for $g=k=0{\cdot}01$ on an IBM 1620 computer as a function of thickness ($\mu t=2gA$) and this is shown in Fig. 1. For very small values of thickness ($\mu t<0{\cdot}001$) we have the linear kinematical region and as the thickness increases ($\mu t\simeq 0{\cdot}03$) we *approach* the maximum or Ewald value of $R^y_H=\pi$ while for very thick crystals ($\mu t>8$) we *approach* the Darwin solution of $\frac{8}{3}$. The approximate criteria for a thick crystal (*i.e.* R^y_H yields the Darwin solution to within 0·1 %) occurs for values of $\mu t\geq 8$.

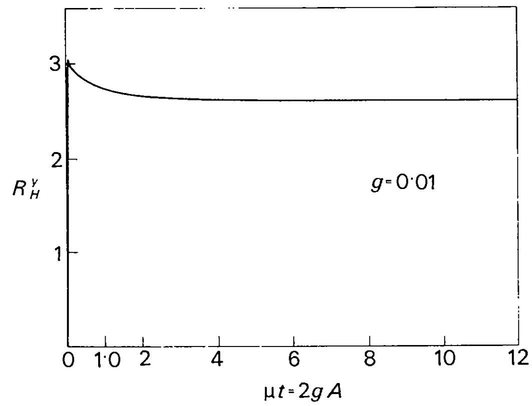

Fig. 1. The integrated intensity $R^y{}_H$ as a function of the product of the absorption coefficient μ and the effective thickness $t(t=t_0/\sin\theta_B)$ for Bragg reflexions of a plane parallel perfect crystal plate, $g=k=0{\cdot}01$. For very small values of μt the integrated intensity approaches the kinematical value which is linear in t while for very large values of μt the curve approaches the Darwin value. For $\mu t\sim 0{\cdot}03$ the integrated intensity approaches the Ewald value. The thick crystal criteria (*i.e.* $R_H{}^y$ yields the Darwin solution to within 0·1 %) occurs for values of μt greater than indicated by the arrow. (Owing to the finite value of g the actual Darwin limit of equation (1) is 2·61 rather than $\frac{8}{3}$ while the peak value is 3·01 rather than π).

It is interesting to note that a thin crystal $\mu t\sim 0{\cdot}03$ gives more integrated intensity than a thick crystal $\mu t>8$, and this presumably arises from interference effects amongst the multiply scattered waves with the front and back surfaces combined with absorption of the multiply scattered waves.

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References

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