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A METHOD FOR DETERMINING THE ANOMALOUS ABSORPTION PARAMETER OF A CRYSTAL

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W. L. Bell and G. Thomas

Inorganic Materials Research Division, Lawrence Radiation Laboratory, and the Department of Mineral Technology, College of Engineering, University of California, Berkeley, California

May 1968

The two-beam dynamical theory gives the intensity diffracted by a perfect wedge-shaped, absorbing crystal at the Bragg angle for diffraction

$$I_{s}(t) = \frac{I_{o}e^{-2At}}{2} (\cosh 2Bt - \cos 2\pi t)$$

where $A = \pi t_0 / \xi_0^{\dagger}$, $B = \pi t_0 / \xi_g^{\dagger}$, and $t = z/t_0$ are all dimensionless parameters of absorption and thickness. In common notation ξ_0^{\dagger} and ξ_g^{\dagger} are the mean and anomalous absorption distances, t_0 is the extinction distance, and z is the thickness of the foil; all are generally expressed in Angstroms.

Values for the absorption parameters are obtained using the extrema values from an intensity profile and determining the envelope for the intensity variations. The mean parameter is obtained from

$$I_{\Delta}(t) = I_{max}(t) - I_{min}(t) = I_{o}e^{-2At}$$
 (2)

and the anomalous parameter from

as:

$$\frac{I_{\Sigma}(t)}{I_{\Delta}(t)} = \frac{I_{\max}(t) + I_{\min}(t)}{I_{\max}(t) - I_{\min}(t)} = \cosh 2Bt \rightarrow \frac{e^{2Bt}}{2} \qquad (3)$$

in thick foils. If there is a diffuse or incoherent background intensity distribution, G(t), Equation (2) will be independent of the background while Equation (3) should contain twice the amount of background present in the image.

All previous methods¹⁻³ of obtaining the anomalous parameter have ignored background radiation and are therefore inherently inaccurate. Using background the following expression can be obtained:

 $\frac{I_{\Sigma}(t) - I_{\Sigma}(t+1)}{I_{\Delta}(t)} = \left[\frac{I_{\Sigma}(t)}{I_{\Delta}(t)}\right] - \left[\frac{I_{\Delta}(t+1)}{I_{\Delta}(t)} \frac{I_{\Sigma}(t+1)}{I_{\Delta}(t+1)}\right]$ $= \cosh 2Bt - e^{-2A} \cosh 2B(t+1) + \frac{\Delta G}{I_{0}e^{-2At}}$

where $\Delta G = 2G(t) - 2G(t+1)$. Both the sign and the magnitude of ΔG will depend upon the shape of the background curve and the thicknesses used in Equation (4). Using two thicknesses before the maximum in the background distribution curve, 2B calculated by Equation (4), ignoring background (i.e., assuming $\Delta G = 0$), will be an overestimate; points used past this maximum will yield a value of 2B which is an underestimate when background is ignored. The simplest application is therefore to obtain the background distribution and determine its maximum. The interpolated value of the anomalous parameter at this thickness will be quite close to the real value. An alternate method would be to obtain two micrographs of the same wedgeshaped foil using different amounts of divergent radiation and hence different percentages of diffuse background intensities contributing to the images. The plots of the anomalous absorption parameters versus thickness

obtained for the two cases will then cross at the correct value of the parameter and at a thickness approximately where the background exhibits a maximum.

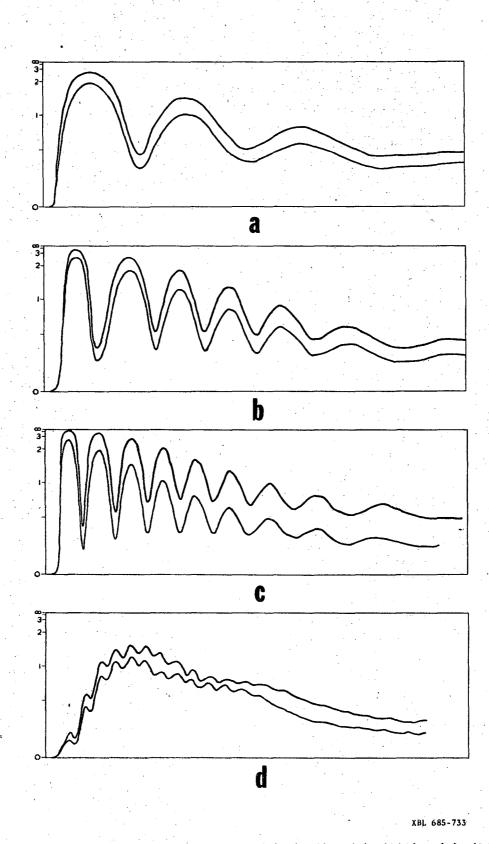
Figure 1 shows the microphotometer traces obtained for two different amounts of defocusing the condenser lens on the Siemens I microscope, from the aluminum foil shown in Figure 2, and the intensity distribution at the (111) reciprocal lattice point when the angle of incident radiation is far from the Bragg angle. The values of the anomalous parameter determined by Equation (4), ignoring background, are shown in Figure 3, and it can be seen that the curves for different background distributions cross at thicknesses quite close to the observed maximum in the background distributions. Points on the plots are all relative to the (111) extinction distance and therefore these results show that the anomalous absorption length is not constant but varies with diffracting planes. However, these results indicate that the ratio of the imaginary part of the Fourier coefficient of the lattice potential to the real part is 0.431 for the (111) planes and 0.453 for the (200) planes in aluminum and that this ratio is fairly constant.

ACKNOWLEDGMENTS.

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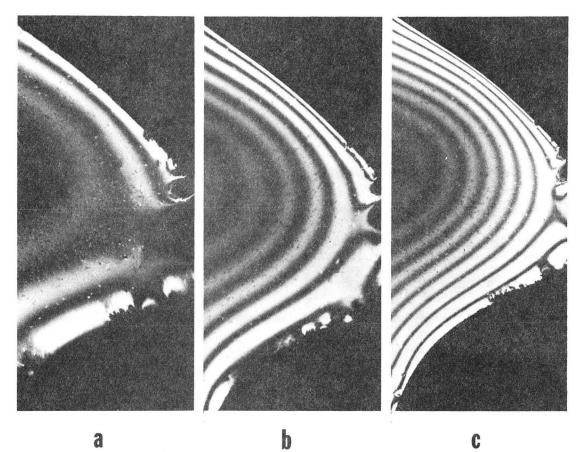
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Fig. 1 Microphotometer traces for (a) (220), (b) (002), (c) (111) planes diffracting in aluminum and (d) the diffuse background distribution for the (111) reflection far from the Bragg angle.

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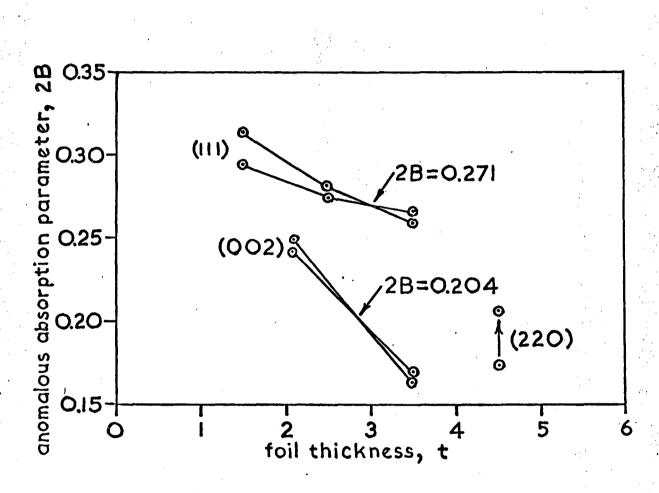


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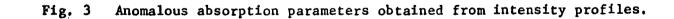
Fig.2

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Fig. 2 Electron micrographs of Al foil for (a) (220), (b) (002) and (c) (111) plane's diffracting.



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