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# Numerical Methods in the Theory of Diffraction Contrast of Crystal Lattice Defects

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Following the methods originally given by Darwin[1], it has recently been possible to find a very simple representation of the equations describing the dynamical equilibrium between incident and diffracted beams in the Laue case (Howie and Whelan[2], Howie[3], for a full discussion see Howie and Whelan[4),5]). In the two-beam case the equations are best expressed in the form of coupled linear differential equations

$$\left.\begin{aligned}\frac{dT}{dz}&=i\frac{\pi}{\xi_g}S\,,\\ \frac{dS}{dz}&=i\frac{\pi}{\xi_g}T+2\pi i s_g S\,,\end{aligned}\right\} \qquad (1)$$

where $z$ is depth in the crystal, $T$ and $S$ are amplitudes of incident and diffracted waves in the crystal, $s_g$ is the distance of the reciprocal lattice point $g$ (corresponding to the reflection) from the reflecting sphere (reckoned positive if the reciprocal lattice point is inside the reflecting sphere), $\xi_g$ is the extinction distance ($\lambda E/V_g$). Several forms of equations (1) can be obtained by making suitable phase transformations on $T$ and $S$, but all predict the same intensities.

The solutions of equations (1) at depth $t$ in the crystal, starting with $T=1$, $S=0$, at the top surface, are the well known Laue solutions for a plate crystal of thickness $t$[4]. Furthermore the equations are easily extended phenomenologically to cover absorption (inelastic scattering), displacements $\boldsymbol{R}(z)$ of atoms near a defect on the 'column approximation' (Hirsch, Howie and Whelan[6]), and several diffracted beams. Absorption is included in the theory by allowing the Fourier coefficients of the lattice potential to become complex, i.e. by replacing $1/\xi_g$ in (1) by $1/\xi_g+i/\xi_g'$, where $\xi_g'$ is a parameter determining the extent of anomalous absorption, and by including a mean absorption coefficient determined by a parameter $\xi_0'$. For the two-beam theory the following quations hold[4]

$$\left.\begin{aligned}\frac{dT}{dz}&=-\frac{\pi}{\xi_0'}T+\pi\left(\frac{i}{\xi_g}-\frac{1}{\xi_g'}\right)S\,,\\ \frac{dS}{dz}&=\pi\left(\frac{i}{\xi_g}-\frac{1}{\xi_g'}\right)T\\ &\quad+\left(-\frac{\pi}{\xi_0'}+2\pi i(s_g+\beta_g')\right)S\,,\end{aligned}\right\} \qquad (2)$$

where

$$\beta_g'=\frac{d}{dz}(\boldsymbol{g}\cdot\boldsymbol{R}(z))\,, \qquad (3)$$

is the term taking account of atomic displacements.

For a perfect crystal ($\beta_g'=0$) equations (2) predict correctly the anomalous absorption effect near the reflecting position[4]. The theory has been generalised to cover the case of several diffracted beams using well known matrix methods (Sturkey[7], Niehrs[8], Fujimoto[9]). It has been shown[4] that the generalisation of equations (2) can be written in the form

$$\frac{d}{dz}\boldsymbol{v}=2\pi i(\boldsymbol{A}+\boldsymbol{\beta}_{g'\mathrm{Diag.}})\boldsymbol{v}\,, \qquad (4)$$

where $\boldsymbol{v}(z)$ is a column vector whose elements are the wave amplitudes, where $\boldsymbol{\beta}_{g'\mathrm{Diag.}}$ is a diagonal matrix whose elements are given by (3), and where $\boldsymbol{A}$ is a matrix whose elements are

$$\left.\begin{aligned}A_{gg}&=s_g+\frac{i}{2\xi_0'}\,,\\ A_{gh}&=\frac{1}{2}\left(\frac{1}{\xi_{g-h}}+\frac{i}{\xi_{g-h}'}\right).\end{aligned}\right\} \qquad (5)$$

Equations (2) and (4) are well suited to solution by numerical methods. Standard programmes for the EDSAC 2 digital computer at the Mathematical Laboratory, Cambridge, have therefore been used to calculate electron microscope images of various types of dislocation configurations in thin foils. In a typical case several parameters must be specified in the calculation. We must know the absorption parameters $\xi_0'$ and $\xi_g'$. Hashimoto, Howie and Whelan[10] have shown by studies

of extinction contours and fringes at stacking faults that $\xi_g/\xi_g' \sim 0.1$, $\xi_g' \sim \xi_0'$ in a typical metal. Values of this order have been used in all calculations. Parameters describing the particular defect configuration must also be specified, e.g. the quantity $\boldsymbol{g}\cdot\boldsymbol{b}$[6] ($\boldsymbol{b}$=Burgers vector of dislocation), $y/\xi_g$ (its depth below the top surface), $t/\xi_g$ (the crystal thickness), the deviation parameter $w=\xi_g s_g$ of the dynamical theory, etc.

Fig. 1 (a) and (b) shows bright field (BF) and dark field (DF) images of screw and edge dislocations ($\boldsymbol{g}\cdot\boldsymbol{b}=1$) in the middle of a foil of $t=8\xi_g$ (see inset diagram) for $w=0$, com-

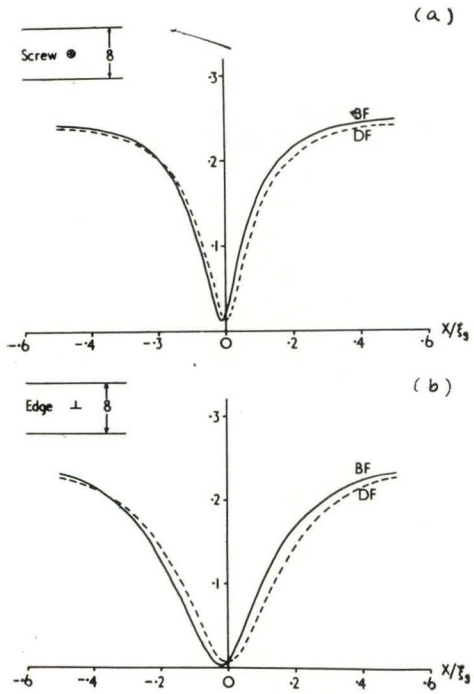


Fig. 1.

puted on the two-beam theory. With the chosen absorption parameter, the foil thickness is sufficient to cause dark field and bright images of dislocations to appear similar in contrast to the complementary behaviour observed when no absorption occurs. The width of the image of a screw dislocation is $\sim\xi_g/5$, while the edge dislocation appears wider. Both these effects were predicted by qualitative arguments in a previous kinematical theory[6]. Other configurations of edge dislotions have been studied by Howie and Whelan[5].

Images of partial dislocations have also been studied. Here $\boldsymbol{g}\cdot\boldsymbol{b}=0$, $\pm 1/3$, $\pm 2/3$ etc., and a stacking fault occurs on one side of the dislocation. Fig. 2 shows computed bright field images for the cases $\boldsymbol{g}\cdot\boldsymbol{b}=1/3$ and $-2/3$ ($y/\xi_g=1.225$, $t/\xi_g=7.25$, $\xi_g/\xi_g'=0.075$, $w=-0.2$). The broken line on the left is the level of intensity in the perfect crystal; that on the right is the level in the faulted crystal. The computations show that partials with $\boldsymbol{g}\cdot\boldsymbol{b}=\pm 1/3$ show little contrast near the edge of the fault and are expected to be invisible. Partials with $\boldsymbol{g}\cdot\boldsymbol{b}=\pm 2/3$ are expected to appear as a dark line. Observations of these contrast effects have been made[5].

The problem of slip trace contrast has also been investigated on the assumption that a moving dislocation leaves a dislocation below the surface of the metal (oxide film trapping).

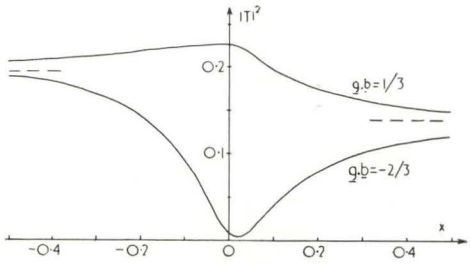


Fig. 2.

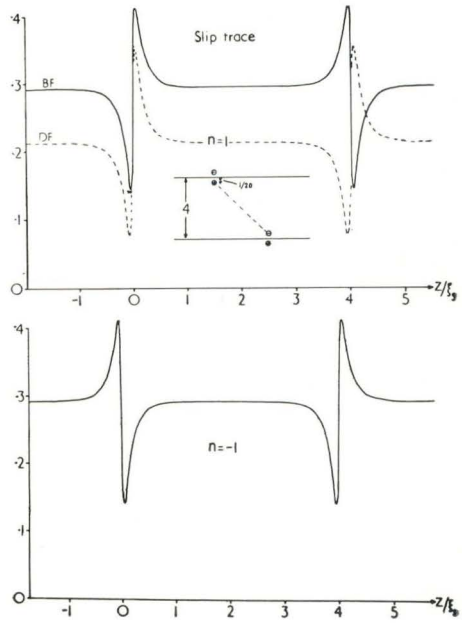


Fig. 3.

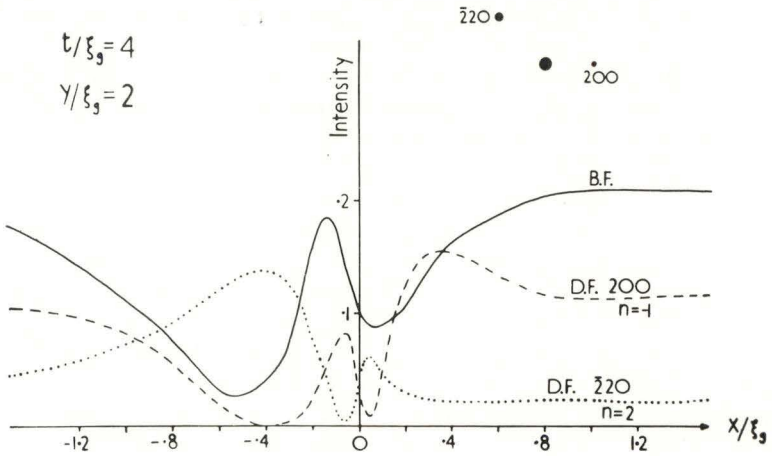


Fig. 4.

Such a dislocation with its image is expected to behave as a dipole, and Fig. 3 shows calculations of the contrast from such dipoles for bright field images (full curves) and dark field images (broken curves) ($t/\xi_g=4$, dipole spacing$=1/10\xi_g$). The bright field image is symmetrical, i.e. both edges of the trace appear similar, while the dark field image is asymmetrical. Similar effects have been reported for stacking fault fringes[10], and they may be used to differentiate between top and bottom surfaces of the foil. The pair of light and dark fringes at the edges of a trace have been observed frequently[5], and are observed to reverse on changing the sign of $\boldsymbol{g}$ by tilting ($n=\boldsymbol{g}\cdot\boldsymbol{b}=1$ and $-1$ in Fig. 3). This dipole theory does not predict appreciable contrast inside a trace as is frequently observed, and this is due to the limitations of the model. Presumably some local buckling of the foil occurs and this is not included in the model.

Several other contrast effects have been investigated including double images on a multiple beam theory. Fig. 4 shows computed bright field and dark field images of a screw dislocation for the case where two strong reflections occur (200 and $\bar{2}20$, see schematic diffraction pattern inset in Fig. 4). It has been possible to explain qualitatively the appearance of double images of a dislocation in bright field, in agreement with the predictions of the kinematical theory[6]. However the number of variable parameters in the multiple beam theory is so large that up to the present time no systematic examination has been attempted.

A complete account of the work reported in this note is being published[4),5)].

This work was carried out in collaboration with Dr. A. Howie, to whom my thanks are due for permission to include joint work. I am also indebted to Dr. P. B. Hirsch for valuable discussions and to the Director of the Mathematical Laboratory, Cambridge, for use of EDSAC 2.

## References

1 C. G. Darwin: Phil. Mag. **27** (1914) 315, 675.
2 A. Howie and M. J. Whelan: *Proc. European Regional Conference on Electron Microscopy, Delft*, **1** (1960) 194.
3 A. Howie: *Report of AIME conference, St. Louis* (in the press),
4 A. Howie and M. J. Whelan: Proc. Roy. Soc. **A263** (1961a) 217.
5 A. Howie and M. J. Whelan: Proc. Roy. Soc. (1961b), in the press.
6 P. B. Hirsch, A. Howie and M. J. Whelan: Phil. Trans. Roy. Soc. **A252** (1960) 499.
7 L. Sturkey: Acta. Cryst. **10** (1957) 858.
8 H. Niehrs: Z. Naturforsch. **14** (1959) 504.
9 F. Fujimoto: J. Phys. Soc. Japan **14** (1959) 1558.
10 H. Hashimoto, A. Howie and M. J. Whelan: Phil. Mag. **5** (1960) 967; Proc. Roy. Soc. (1962), in the press, .

## DISCUSSION

L. STURKEY: (1) The method of Darwin was originally used by me to derive my scattering matrix method (about 1955). If you look at your equations, you will see that they are a simple matrix equation:

$$\frac{\partial}{\partial t}\begin{pmatrix} T \\ S \end{pmatrix} = i\boldsymbol{M}\begin{pmatrix} T \\ S \end{pmatrix},$$

with the usual exponential solution

$$\begin{pmatrix} T \\ S \end{pmatrix} = e^{i\boldsymbol{M}t}\begin{pmatrix} T_0 \\ S_0 \end{pmatrix},$$

where $\boldsymbol{M}$ is the scattering matrix.

(2) If $\xi'_0 \cong \xi'_g$, then this means that the absorption can become positive, i.e. the absorption coefficient can become negative. This means that electrons are created in the lattice. I suggest that you include absorption as indicated in my paper for the "Proceedings" (p. 211).

M. J. WHELAN: (1) I am quite aware of the relations Dr. Sturkey points out and I do not know of any place in the literature where he describes the use of Darwin's method applied to the Laue case.

(2) I am aware of the point Dr. Sturkey has raised. If $\xi_0' = \xi_g'$, (*i.e.* $V_0' = V_g'$) then the complex potential would have to be distributed like a set of $\delta$-functions at the atomic positions, i.e. the inelastic scattering is concentrated at each atom. This distribution is the only one which gives $\xi_0' = \xi_g'$ without becoming negative at some point. Incidentaly, $\xi_0' = \xi_g'$ for all $g$. I only implied that $\xi_0'$ is of the same order as $\xi_g'$. Hashimoto's measurements show that $\xi_0' = 0.6\xi_g'$ roughly. Another point is that in the two-beam theory the image profile of a dislocation etc. is not affected by the value of $\xi_0'$. This parameter only determines the scale of the intensity profile.