Title
NUMERICAL ANALYSIS OF THE MULTIPLE BEAM EQUATIONS FOR ELECTRON DIFFRACTION

Authors
Bell, W.L.
Thomas, G.

Publication Date
1969-04-01

Submitted to 27th Annual EMSA Meeting,
St. Paul, Minnesota, August 26-29, 1969

UCRL-19001
Preprint

cy. 2

NUMERICAL ANALYSIS OF THE MULTIPLE BEAM EQUATIONS FOR ELECTRON DIFFRACTION

W. L. Bell and G. Thomas

April 1969

AEC Contract No. W-7405-eng-48

LAWRENCE RADIATION LABORATORY
UNIVERSITY of CALIFORNIA BERKELEY

UCRL-19001

cy. 2

DISCLAIMER

NUMERICAL ANALYSIS OF THE MULTIPLE BEAM EQUATIONS FOR ELECTRON DIFFRACTION

W. L. Bell and G. Thomas

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

The differential equations of the n-beam dynamical theory of electron diffraction are, neglecting absorption and common phases,

$$\frac{d\psi_i}{dz} = z\pi i\, s_i\, \psi_i + \sum_{\substack{j=0 \\ j\neq i}}^{n-1} \frac{\pi i}{\xi_{j-i}}\, \psi_j\, e^{2\pi i \bar{g}_{j-i}\cdot\bar{R}} \qquad (1)$$

where the subscript i is taken from zero to (n-1) to yield the n differential equations. ψ_0 is the forward diffracted wave and $\psi_1\ \psi_2 \cdots \psi_{n-1}$ are the other (n-1) diffracted waves; s_i is the macroscopic deviation parameter of the i^{th} reciprocal lattice point; $\bar{g}_{j-i}$ is the reciprocal lattice vector connecting the i^{th} and the j^{th} reciprocal lattice points and ξ_{j-i} is the extinction distance corresponding to two-beam dynamical diffraction by the planes for which $\bar{g}_{j-i}$ is the reciprocal lattice vector. For numerical analysis of these equations, Howie and Whelan[1] have suggested the use of alternate wave functions given by

$$\psi_i' = \psi_i\, e^{2\pi i\, \bar{g}_i\cdot\bar{R}} = \psi_i\, e^{2\pi i\beta} \qquad (2)$$

The differential equations then become

$$\frac{d\psi_i'}{dz} = 2\pi i\, (s_i + \beta_i')\, \psi_i' + \sum_{\substack{j=0 \\ j\neq i}}^{n-1} \frac{i\pi}{\xi_{j-i}}\, \psi_j' \qquad (3)$$

where

$$\beta_i' = \frac{d}{dz}\, (\bar{g}_i \cdot \bar{R}). \qquad (4)$$

The matrix representation of this set of equations is

$$\frac{d}{dz} [\psi'] = 2\pi i (A + \{\beta_i'\}) [\psi'] \quad (5)$$

where $[\psi']$ is a column matrix with elements ψ_i. A is the eigenvalue matrix (nxn) for the perfect crystal, and $\{\beta_i'\}$ is an nxn diagonal matrix with elements β_i'. In this form, the equations are suitable for numerical analysis and, for a slab of thickness Δz,

$$[\psi'(z + \Delta z)] = (I + 2\pi i \Delta z (A + \{\beta_i'\})) [\psi'(z)] \quad (6)$$

where I is the nxn identity matrix. Rearranging terms, this becomes

$$[\psi'(z + \Delta z)] = (\{1 + 2\pi i \Delta z (s_i + \beta_i')\} + 2\pi i \Delta z B) [\psi_i(z)] \quad (7)$$

where Bis the nxn matrix $(A-\{s_i\}$ and has zeroes for its elements on the main diagonal. Equation (7) is equivalent to the n equations

$$\psi_i'(z + \Delta z) = \left(1 + 2\pi i \Delta z (s_i + \beta_i')\right)\psi_i'(z) + \sum_{j \neq i} \frac{i\pi \Delta z}{\xi_{j-i}} \psi_j'(z) \quad (8)$$

obtainable directly from equation (3) using incremental equations rather than differential equations. Equation (8) can easily be programmed for a computer if Δz, s_i, β_i', ξ_{j-i} and initial conditions are specified, and repitition of equation (8) m times can be used to obtain the amplitude of ψ_i for a foil of thickness $m\Delta z$. Although the differential equations used to obtain equation (8) are in perfect accord with the dynamical theory, equation (8) itself is not conservative in that the intensity of the i^{th} diffracted beam is multiplied by a factor $[1+(2\pi\Delta z)^2(s_i+\beta_i')^2]$. This is not a serious effect provided Δz is chosen small enough. However, a slab thickness, Δz, suitable for a two beam calculation will be too large for the general multiple beam case, particularly one involving syste-

matic reflections, because of the large values of s_i associated with higher order beams and the large $\bar{g}_i \cdot \bar{b}$ products appearing in β_i'. Also, equation (8) is particularly unsuitable to the situations where β_i' is a δ-function, such as in the cases of stacking faults and antiphase boundaries where $\bar{g} \cdot \bar{R}$ has an abrupt change and in situations involving delta boundaries where the value of s_i changes abruptly. In order to overcome the non-conservative nature of the numerical solution of the dynamical equations, a substitution other than equation (2) can be used. If

$$\psi_i'' = \psi_i \, e^{-2\pi i s_i z} \tag{9}$$

then

$$\frac{d\psi_i''}{dz} = \sum_{j \neq i} \frac{\pi i}{\xi_{j-i}} \psi_j'' \, e^{2\pi i (s_{j-i} z + \bar{g}_{j-i} \cdot \bar{R})} \tag{10}$$

In matrix notation this becomes

$$\frac{d}{dz} [\psi''] = \{e^{-2\pi i (s_i z + \bar{g}_i \cdot \bar{R})}\} (2\pi i B) \{e^{2\pi i (s_i z + \bar{g}_i \cdot \bar{R})}\} \tag{11}$$

where the diagonal matrices are termed "shift" matrices by Amelinckx[2] and B is the same matrix as introduced in equation (7). For a numerical analysis, equation (11) will give

$$[\psi''(z+\Delta z)] = (I + \{e^{-2\pi i (s_i z + \bar{g}_i \cdot \bar{R})}\} (2\pi i \Delta z B) \{e^{2\pi i (s_i z + \bar{g}_i \cdot \bar{R})}\}) [\psi''(z)] \tag{12}$$

If $[\psi''(z)]$ is considered as the waves incident on a crystal slab at depth z, then

$$[\psi(z)] = \{e^{2\pi i (s_i z + \bar{g}_i \cdot \bar{R})}\} [\psi''(z)] \tag{13}$$

might be considered as waves transformed upon entering the slab, and

$$[\psi'(z+\Delta z)] = \{e^{2\pi i (s_i \Delta z + \bar{g} \cdot \Delta \bar{R})}\} (I + 2\pi i \Delta z B) [\psi'(z)]. \tag{14}$$

The corresponding system of equations is then

$$\psi_i'(z+\Delta z) = e^{2\pi i(s_i\Delta z+\bar{g}_i\cdot\Delta\bar{R})}\left[\psi_i'(z) + \sum_{j\neq i}\frac{i\pi\Delta z}{\xi_{j-i}}\psi_j'(z)\right]. \qquad (15)$$

These equations can also be handled easily by a computer provided the exponential functions can be defined conveniently. The primary advantage of using equation (15) rather than equation (8) is the elimination, for the most part, of the non-conservative nature of the numerical solution. ψ_i' is the same wave function in both equations, i.e., equations (9) and (13) equal equation (2). Furthermore, for small phase angles, $2\pi i(s_i\Delta z+g_i\cdot\Delta R)$, equation (15) can be converted into equation (8), if terms involving $(\Delta z)^2$ are neglected, since

$$\bar{g}\cdot\Delta\bar{R} \cong \frac{d}{dz}(\bar{g}\cdot\bar{R})\Delta z. \qquad (16)$$

The modified wave functions, ψ_1' were defined for equation (15) after numerical approximations to the differentials equations where made rather than before, and the result was a greater degree of conservation of electron intensity than is possible with equation (8).

Absorption has been neglected for simplicity's sake, but it can be introduced easily into equation (15) by representing mean absorption in a slab as a coefficient of the exponential function and anomalous absorption can be duplicated by replacing the reciprocals of the extinction distances with suitable real and imaginary terms.

Acknowledgements

We wish to thank the United States Atomic Energy Commission for continued financial support of the research.

REFERENCES

1. Hirsch, P. B., Howie, A., Nicholson, R.B., Pashley, D. W., and Whelan, M.J., Electron Microscopy of Thin Crystals (Butterworths, London, 1965).

2. Amelinckx, S., The Direct Observation of Dislocations (Academic Press, New York, 1964).

LEGAL NOTICE

TECHNICAL INFORMATION DIVISION
LAWRENCE RADIATION LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720