Title
A COMPUTATIOHAL METHOD FOR IMAGE ANALYSIS OF A CRYSTAL CONTAINING DEFECTS

Authors
Tan, T.Y.
Bell, W.L.

Publication Date
1971-04-01

Presented at 29th Annual EMSA Meeting,
Boston, Mass. August 9-13, 1971

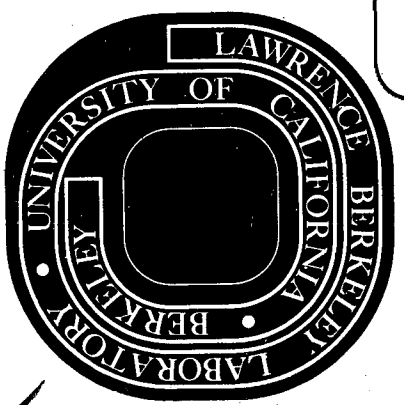
UCRL-20560
Preprint

A COMPUTATIONAL METHOD FOR IMAGE ANALYSIS OF A CRYSTAL CONTAINING DEFECTS

T. Y. Tan and W. L. Bell

April 1971

AEC Contract No. W-7405-eng-48



UCRL-20560

DISCLAIMER

A COMPUTATIONAL METHOD FOR IMAGE ANALYSIS OF A CRYSTAL CONTAINING DEFECTS

T. Y. Tan and W. L. Bell

Department of Materials Science and Engineering, University of California, Berkeley, California 94720

Within the scope of column approximation, image analysis of crystals containing defects amounts to solving the set of linear differential equations for all appreciably excited Bragg beams: (1)

$$\frac{d}{dz}\underset{\sim}{\Psi}'_h(\bar{r}) = \underset{\approx}{A}'_R\,\underset{\sim}{\Psi}'_h(\bar{r}) \qquad (1)$$

where

$$\underset{\approx}{A}'_R = 2\pi i \begin{bmatrix} k_r + S_0 & \frac{1}{2\xi_{g_1}} & \cdots & \frac{1}{2\xi_{g_n}} \\ \frac{1}{2\xi_{g_1}} & k_r + S_{g_1} + \frac{d}{dz}\bar{g}_1\cdot\bar{R} & \cdots & \\ \vdots & & \ddots & \\ \frac{1}{2\xi_{g_n}} & \cdots\cdots & & k_r + S_{g_n} + \frac{d}{dz}\bar{g}_n\cdot\bar{R} \end{bmatrix}$$

(here all quantities have their usual definitions as in the literatures). Within a thin slice $\Delta z_m = z_m - z_{m-1}$ where $\bar{R}(\bar{r})$ can be approximated as a constant $\bar{R}_m$, then Eq. (1) has the solution

$$\underset{\sim}{\Psi}'_h(z_m) = e^{\underset{\approx}{A}'_{R_m}\Delta z_m}\,\underset{\sim}{\Psi}'_h(z_{m-1}). \qquad (2)$$

A conventional method of solving the image problem utilizes Eq. (2) and an approximate series expansion form of the dispersion matrix, i.e., $\underset{\approx}{\Phi}(\Delta z_m) = e^{\underset{\approx}{A}'_R\Delta z_m} \approx \underset{\approx}{I} + \underset{\approx}{A}'_R\Delta z_m$. This method suffers from two major shortcomings: 1) it requires very long computing time, since now Δz_m has to be kept as very small, 2) due to the presence of the terms $S_h + d(\bar{h}\cdot\bar{R})/dz$ in the diagonal elements in the matrix $\underset{\approx}{A}'_R$, the total electron intensity (aside from the parts due to absorptions) is not conserved, since now the quantity S_h can be very large for high order beams and on crossing slices with an abrupt change in $\bar{R}$ (e.g., stacking faults and antiphase boundaries), $d(\bar{h}\cdot\bar{R})/dz$ may become a δ-function. To avoid the second difficulty it is necessary to solve the problem as a standard eigenvalue problem slicewise. This method is, however, even more time consuming. We present in this paper a method which retains the mathematical rigor of the eigen-solution method yet simultaneously considerable amount of computing time can be saved. Eq. (1) may be written in a slight different form to yield

$$\underset{\sim}{\Psi}_h(z) = e^{\underset{\approx}{A}_{R_m}\Delta z_m}\,\underset{\sim}{\Psi}(z_{m-1}) \qquad (3)$$

with

$$\underset{\approx}{A}_{R_m} = 2\pi i \begin{bmatrix} k_r + S_0 & \frac{e^{\alpha_{g_1}}}{2\xi_{g_1}} & \cdots & \frac{e^{\alpha_{g_n}}}{2\xi_{g_n}} \\ \frac{e^{-\alpha_{g_1}}}{2\xi_{g_1}} & k_r + S_{g_1} & \cdots & \\ \vdots & & \ddots & \\ \frac{e^{-\alpha_{g_n}}}{2\xi_{g_n}} & \cdots\cdots & & k_r + S_{g_n} \end{bmatrix}$$

where $\alpha_{g_\ell} = 2\pi i\,\bar{g}_\ell\cdot\bar{R}_m$.

It is a straight forward matter to show that

$$\det.\,(\underset{\approx}{A}_{R_m} - \lambda\,\underset{\approx}{I}) = \det.\,(\underset{\approx}{A}_{R=0} - \lambda\,\underset{\approx}{I}). \qquad (4)$$

Eq. (4) implies that the eigenvalues of A_R and hence that of $\underset{\approx}{\Phi}(R_m, \Delta z_m)$ are indepent of $\bar{R}_m$ and are just those of the perfect crystal. However, for slices having different values of $\bar{R}$, their corresponding eigenvectors must change. It is also easily seen that in a slice of displacement $\bar{R}_m$ and thickness Δz_m,

$$\underset{\approx}{\bar{\Phi}}(\bar{R}_m, \Delta z_m) = \underset{\approx}{T}^{-1}_{R_m} \underset{\approx}{\bar{\Phi}}(0, \Delta z_m) \underset{\approx}{T}_{R_m} \qquad (5)$$

where $$\underset{\approx}{T}_{R_m} = \left[e^{2\pi i \bar{g}_{p-1} \cdot \bar{R}_m} \delta_{pr} \right].$$

The above discussions suggest that once the dispersion matrix for the perfect crystal is found and with the computed results kept in the wave forms, then that of any slice of a deformed crystal can be obtained by Eq. (5), which involves only two matrix multiplications. The waves leaving one slice is simply obtained by multiplying the dispersion matrix by the waves entering this slice. Upon iterating through the crystal, even further simplifications occur: At the exit surface of the crystal of thickness t

$$\underset{\sim}{\psi}_h(t) = \underset{\approx}{T}^{-1}_{R_j} \underset{\approx}{\bar{\Phi}}(0, \Delta z_j) \underset{\approx}{\hat{T}}_{\Delta R_j} \underset{\approx}{\bar{\Phi}}(0, \Delta z_{j-1}) \cdots \underset{\approx}{\hat{T}}_{\Delta R_1} \underset{\approx}{\bar{\Phi}}(0, \Delta z_1) \underset{\approx}{T}_{R_1} \underset{\sim}{\psi}_h(0) \qquad (6)$$

where

$$\underset{\approx}{\hat{T}}_{\Delta R_m} = \underset{\approx}{T}_{R_m} \underset{\approx}{T}^{-1}_{R_{m-1}} = \left[e^{2\pi i (\bar{R}_m - \bar{R}_{m-1}) \cdot \bar{g}_{p-1}} \delta_{pr} \right],$$

just a single matrix.

Because this method is a modified eigen-solution method based on the special property of the scattering matrix [Eq. (4)], thus on one hand it naturally avoided all the difficulties associated with the fundamental incremental method, yet on the other hand considerable amount of computing time can be saved in comparison with the standard eigen-solution method. This is so because in general if the standard eigen-solution method amounts to solve j eigenvalue problems for the j slices of the crystal, this method converts it into a task of solving one eigenvalue problem plus 2j simple matrix multiplications. It may be further noticed that the accuracy of the solution depends only upon the incremental displacement $\Delta \bar{R}_m$, not Δz_m.

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

This work is supported by the U.S. Atomic Energy Commission through the Lawrence Radiation Laboratory, Berkeley, California 94720.

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