THE RECONSTRUCTION OF DISPLACEMENT FIELDS OF DEFECTS IN CRYSTALS FROM ELECTRON MICROGRAPHS

I. ANALYTIC FIELDS

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[*Manuscript received July* 24, 1968]

Summary

The following theorem and corollaries are proved. If the two-beam column approximation theory of electron microscope image formation is assumed and if the displacement field of the object is analytic with zero derivative at infinity, and such that there is a direction in the object along which displacements are constant, then from an electron micrograph that records intensities but no phase information there is an explicit and unique reconstruction of the component of the displacement field of the object in the direction of the diffracting vector, except possibly in some specified singular cases for which the reconstruction cannot be started uniquely.

The vector displacement field can be reconstructed from three micrographs taken with non-coplanar diffracting vectors.

Three micrographs taken with non-coplanar diffracting vectors uniquely identify a defect.

Bright field and dark field micrographs contain identical information since either can be used for reconstruction.

If two micrographs have identical intensity distribution then they have identical phase distribution.

A blank micrograph can only be from a null displacement component field.

I. Introduction

With the introduction of the computer generation of electron micrographs of defects in crystals (Head 1967; Humble 1968) there has come a fuller realization of the many and varied types of image that any particular class of defect, e.g. dislocations, can have. One immediate use of this variety has been the identification of defects by the matching of experimental images taken under a range of experimental conditions against a corresponding range of theoretical pictures for a number of possible defects which, it is hoped, includes the unknown object. It has usually been possible by this trial and error method to identify a defect by elimination, i.e. for all trial defects except one, at least one theoretical picture is in obvious disagreement with the corresponding experimental picture. However, this does not really prove the identification, for there might be another defect that was not considered which would also have a set of theoretical pictures that would match. This is particularly so as an electron micrograph only records intensities and not phases so that there is the apparent possibility of two defects giving identical intensity distributions but different phase distributions.

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II. Basic Theorem

As an initial step in the examination of the question of the uniqueness of electron micrographs, the following theorem is proved in this paper.

If (i) *the two-beam column approximation theory of electron microscope image formation is assumed and if the displacement field* $\boldsymbol{R}$ *of the object is* (ii) *analytic with zero derivative at infinity and* (iii) *such that there is a direction in the object along which displacements are constant, then from an electron micrograph that records intensities but no phase information there is an explicit and unique reconstruction of the component of the displacement field of the object in the direction of the diffracting vector* $\boldsymbol{g}$, *except possibly in some specified singular cases for which the reconstruction cannot be started uniquely.*

The assumption (i) of an approximate theory means that this therorem is only strictly true for computer-generated micrographs which have been calculated using just this theory. Any application to experimental micrographs will depend on how good an approximation this theory really is.

The assumption (iii) is equivalent to restricting consideration to displacement fields for which a generalized cross section can be defined (Head 1967; Humble 1968). All the types of computed micrographs in Head (1967) and Humble (1968), covering a range of dislocation and stacking fault configurations, would therefore be included.

The assumption (ii) will be considered in more detail in Section V. It will include dislocations but exclude stacking faults, since the displacement fields of the latter have arbitrary discontinuities and are not analytic.

III. Image Formation

The method that has been used (Head 1967) in the calculation of theoretical micrographs of displacement fields satisfying assumption (iii) above suggests that there is a close relationship between intensities along each line of the picture that is parallel to the projection of the constant direction. In this section we consider a transformation of the differential equations of Howie and Whelan (1961) describing image formation, into a form that emphasizes this relationship.

The Howie–Whelan equations for ϕ_0 and ϕ_g, the amplitudes of the direct and diffracted beams, can be written in many equivalent ways (e.g. Hirsch *et al.* 1965), and for simplicity of analysis we take the following form.

$$\frac{\mathrm{d}\phi_0}{\mathrm{d}z} = Q\phi_g\,, \qquad \frac{\mathrm{d}\phi_g}{\mathrm{d}z} = Q\phi_0 + \mathrm{i}\left(2w + 2\pi\frac{\mathrm{d}\beta}{\mathrm{d}z}\right)\phi_g\,, \tag{1}$$

where

$$Q = \mathrm{i} - \xi_g/\xi_g'\,, \qquad w = s_g\,\xi_g\,, \qquad \beta(z) = \boldsymbol{g}\,.\,\boldsymbol{R}(z)\,,$$

and the unit of length is ξ_g/π.

Anomalous absorption is included in Q but normal absorption is ignored as, initially, specimens of constant thickness t are to be considered and normal absorption will just multiply amplitudes by a constant factor $\exp(-t\xi_g/\xi_0')$.

In Figure 1 is shown a longitudinal section through an untilted parallel-sided object. This section plane is defined as that containing the beam direction and the constant direction of the displacement field $\boldsymbol{R}$ of the object. This plane becomes one line of the picture by projection in the direction of the electron beam. The classical method of image computation is to calculate the intensity at a point on this picture

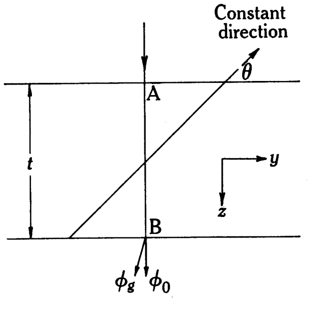

Fig. 1.—Longitudinal cross section of parallel-sided untilted object of thickness t. The constant direction of the displacement field is indicated.

line by integrating the equations (1) down the column, such as AB, which projects into the image point, starting at A with an incident beam $\phi_0 = 1$, $\phi_g = 0$ and finishing at B with bright field intensity $I = \phi_0\phi_0^*$ and dark field intensity $J = \phi_g\phi_g^*$.

Suppose $\mathbf{P}(y)$ is the scattering matrix of the column AB at y, that is,

$$\mathbf{P}(y) = \begin{bmatrix} P_{00}(y) & P_{0g}(y) \\ P_{g0}(y) & P_{gg}(y) \end{bmatrix} \tag{2}$$

and

$$\begin{pmatrix} \phi_0 \\ \phi_g \end{pmatrix}_{\text{out}} = \mathbf{P}(y)\begin{pmatrix} \phi_0 \\ \phi_g \end{pmatrix}_{\text{in}}, \tag{3}$$

and, for convenience, suppose that the unit of length in the y direction is taken as $(\cot\theta)\xi_g/\pi$ so that $\mathrm{d}y/\mathrm{d}z = -1$ along the constant direction of the displacement field.

Then the scattering matrix $\mathbf{P}(y+\delta y)$ of a neighbouring column at $y+\delta y$ is given by

$$\mathbf{P}(y+\delta y) = \begin{bmatrix} 1 & Q\delta y \\ Q\delta y & 1+\mathrm{i}\,\delta y\{2w+2\pi\beta'(y)\} \end{bmatrix} \times \mathbf{P}(y)$$
$$\times \begin{bmatrix} 1 & Q\delta y \\ Q\delta y & 1+\mathrm{i}\,\delta y\{2w+2\pi\beta'(y-t)\} \end{bmatrix}^{-1}, \tag{4}$$

i.e. the displacements in the column at $y+\delta y$ are the displacements in the column at y with the addition of material at the bottom surface of thickness δz ($= \delta y$) which contains displacements $\beta(y)$ and the removal from the top surface of δz of material with displacements $\beta(y-t)$, this notation indicating that the latter was at the bottom surface at $y-t$.

On passing to the limit $\delta y \to 0$, equation (4) gives the following differential equations for the components of $\mathbf{P}$, with a prime denoting differentiation with respect to y.

$$\left.\begin{aligned} P'_{00} &= Q(P_{g0}-P_{0g}), \\ P'_{0g} &= Q(P_{gg}-P_{00}) - P_{0g}\,\mathrm{i}\{2w+2\pi\beta'(y-t)\}, \\ P'_{g0} &= Q(P_{00}-P_{gg}) + P_{g0}\,\mathrm{i}\{2w+2\pi\beta'(y)\}, \\ P'_{gg} &= Q(P_{0g}-P_{g0}) + P_{gg}\,2\pi\mathrm{i}\{\beta'(y)-\beta'(y-t)\}. \end{aligned}\right\} \tag{5}$$

Integration of these equations would give the bright field intensity

$$I(y) = P_{00}P^*_{00}$$

and dark field intensity

$$J(y) = P_{g0}P^*_{g0}$$

along one line of the picture, knowing $\beta(y)$ the component of the displacement field $\boldsymbol{R}$ in the direction of the diffracting vector $\boldsymbol{g}$, specified as a function of y along the bottom of the section.

To start the integration it is necessary to know initial values of $\mathbf{P}$ at some y. One choice could be a column which is known to pass through undistorted crystal for which

$$\left.\begin{aligned} P_{00} &= \frac{1}{\alpha_2-\alpha_1}\Big(\alpha_2\exp(\alpha_1 t) - \alpha_1\exp(\alpha_2 t)\Big), \\ P_{0g} = P_{g0} &= \frac{Q}{\alpha_2-\alpha_1}\Big(-\exp(\alpha_1 t) + \exp(\alpha_2 t)\Big), \\ P_{gg} &= \frac{1}{\alpha_2-\alpha_1}\Big(-\alpha_1\exp(\alpha_1 t) + \alpha_2\exp(\alpha_2 t)\Big), \end{aligned}\right\} \tag{6}$$

where

$$\alpha_{1,2} = \mathrm{i}w \pm (Q^2-w^2)^{\frac{1}{2}}.$$

There is one explicit integral satisfying (5) which is given by

$$P_{00}P_{gg} - P_{0g}P_{g0} = \exp[2\mathrm{i}wt + 2\pi\mathrm{i}\{\beta(y)-\beta(y-t)\}]. \tag{7}$$

IV. Object Reconstruction

The previous section considered the generation of an image function $I(y)$ from a displacement component function $\beta(y)$. The problem of reconstructing the function $\beta(y)$ from a given $I(y)$ is now considered and it is assumed that all parameters (such as thickness, anomalous absorption, deviation from the Bragg condition, etc.) are known but that all that is known about the displacement field is that assumptions (ii) and (iii) of the basic theorem are true.

Referring to Figure 1, suppose that the process of reconstruction started at $y = -\infty$ and is proceeding in the direction of increasing y and has reached AB. Then the only quantity that is not known in the differential equations (5) is $\beta(y)$, the unknown displacement component which is just entering the lower surface. The quantity $\beta(y-t)$ is of course known since it was determined when it entered the lower surface at $y-t$.

A relationship connecting $\beta(y)$ and the known $I(y)$ can be derived, starting with the definition

$$I(y) = P_{00}\overset{*}{P}_{00}.$$

Differentiating with respect to y gives

$$\begin{aligned} I' &= P_{00}\overset{*}{P}{}'_{00} + P'_{00}\overset{*}{P}_{00} \\ &= P_{00}\,Q^*(\overset{*}{P}_{g0} - \overset{*}{P}_{0g}) + \overset{*}{P}_{00}\,Q(P_{g0} - P_{0g}), \end{aligned}$$

on using the differential equations (5) to eliminate the derivatives.

A further differentiation and elimination of derivatives gives

$$\begin{aligned} I'' = {} & 2QQ^*(P_{g0} - P_{0g})(\overset{*}{P}_{g0} - \overset{*}{P}_{0g}) + 2Q^2\overset{*}{P}_{00}(P_{00} - P_{gg}) + 2Q^{*2}P_{00}(\overset{*}{P}_{00} - \overset{*}{P}_{gg}) \\ & + 2iw\{Q\overset{*}{P}_{00}(P_{g0} + P_{0g}) - Q^*P_{00}(\overset{*}{P}_{g0} + \overset{*}{P}_{0g})\} \\ & + 2\pi i\beta'(y)\{Q\overset{*}{P}_{00}P_{g0} - Q^*P_{00}\overset{*}{P}_{g0}\} + 2\pi i\beta'(y-t)\{Q\overset{*}{P}_{00}P_{0g} - Q^*P_{00}\overset{*}{P}_{0g}\}. \end{aligned} \tag{8}$$

Provided the coefficient of $\beta'(y)$ in (8) is not zero (and this possibility is considered in the next section) then this equation can be solved for $\beta'(y)$. If this expression for $\beta'(y)$ is substituted in (5) then the resulting set of differential equations can be used for reconstruction of the scattering matrix $\mathbf{P}$ as a function of y and so of $\beta'(y)$ from (8). Since it is assumed that $\beta'(y) = 0$ at infinity, the initial values of $\mathbf{P}$ at $y = -\infty$ will be given by (6).

It is also possible to reverse the direction of reconstruction by starting at $y = +\infty$ and moving to the left. In this case $\beta'(y)$ is known, having already been reconstructed, and $\beta'(y-t)$ is unknown. But (8) can be used in the same way to eliminate $\beta'(y-t)$ from (5) to give another suitable set of differential equations.

In a similar manner, starting with the dark field intensity

$$J(y) = P_{g0}\overset{*}{P}_{g0},$$

two differentiations give

$$\begin{aligned} J'' = {} & 2QQ^*(P_{00} - P_{gg})(\overset{*}{P}_{00} - \overset{*}{P}_{gg}) + 2Q^2\overset{*}{P}_{g0}(P_{g0} - P_{0g}) + 2Q^{*2}P_{g0}(\overset{*}{P}_{g0} - \overset{*}{P}_{0g}) \\ & + 2iw\{Q^*P_{g0}(\overset{*}{P}_{00} - \overset{*}{P}_{gg}) - Q\overset{*}{P}_{g0}(P_{00} - P_{gg})\} \\ & + 2\pi i\beta'(y-t)\{Q\overset{*}{P}_{g0}P_{gg} - Q^*P_{g0}\overset{*}{P}_{gg}\} + 2\pi i\beta'(y)\{Q^*P_{g0}\overset{*}{P}_{00} - Q\overset{*}{P}_{g0}P_{00}\} \end{aligned} \tag{9}$$

and this too can be used to eliminate either $\beta'(y)$ or $\beta'(y-t)$ from the differential equations (5).

V. Singular Points

The method of reconstruction that has been described comes to an indeterminate situation if the appropriate coefficient of β' in (8) or (9) becomes zero. There are therefore four different cases for such a singular point in the reconstruction:

$$\left.\begin{array}{ll} \text{Bright field, } y \text{ increasing,} & QP^*_{00}P_{g0} - Q^*P_{00}P^*_{g0} = 0\,. \\ \text{Bright field, } y \text{ decreasing,} & QP^*_{00}P_{0g} - Q^*P_{00}P^*_{0g} = 0\,. \\ \text{Dark field, } y \text{ increasing,} & QP^*_{g0}P_{00} - Q^*P_{g0}P^*_{00} = 0\,. \\ \text{Dark field, } y \text{ decreasing,} & QP^*_{g0}P_{gg} - Q^*P_{g0}P^*_{gg} = 0\,. \end{array}\right\} \quad (10)$$

We first consider the possibility that a singular point occurs after a finite amount of β' has been reconstructed. Then if β' is a predictable function, i.e. if its behaviour for all y can be predicted knowing its behaviour over any finite interval, the reconstruction is theoretically complete. The predictable functions of a real variable are the analytic functions, i.e. the function and all its derivatives exist for all y and in addition it can be expressed as a Taylor series expansion about every y. For example, a dislocation gives an analytic function except for the picture line that goes exactly along the core, but in fact it is even simpler, for β' is a rational function of y and the form of the function is known to be the ratio of a polynomial of the fifth degree to a polynomial of the sixth degree. There are thus 12 constants to be determined and this can be done if β' is known at just 12 points. In general if it is assumed that β' (and therefore β) is an analytic function, the possible occurrence of a singular point during reconstruction does not destroy the uniqueness of the reconstruction.

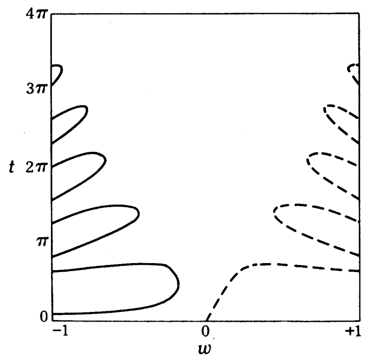

Fig. 2.—Singular combinations of t and w for undistorted crystal and anomalous absorption $\xi_g/\xi'_g = 0\cdot 1$:
—— Bright field for both y increasing and y decreasing.
– – – Dark field for y decreasing.
Dark field for y increasing is given by the mirror image of the dashed curves about $w = 0$. t is in units of ξ_g/π.

A second possibility is that the reconstruction cannot even be started because of a singular point, i.e. the initial values of $\mathbf{P}$ for an undistorted crystal (equations (6)) cause the appropriate coefficient (10) to be zero. It will be seen that both bright field coefficients will be zero together, since for this case $P_{0g} = P_{g0}$. The parameters that are involved are t, w, and the anomalous absorption ξ_g/ξ'_g. If the anomalous absorption is zero then all four conditions of (10) are satisfied simultaneously for the same combinations of t and w, which are (i) for all t if $w = 0$, and (ii) for $t(1+w^2)^{\frac{1}{2}} = n\pi$ with n an integer. For the more typical case $\xi_g/\xi_g' = 0\cdot 1$, Figure 2 shows the combinations of t and w that give singular starting values. It will be seen that they are well away from the combinations that are normally used in practice.

VI. Discussion

We have now essentially proved the theorem since we have shown that, from one line of the micrograph, the longitudinal section of the displacement component field which projects into it can be reconstructed explicitly and uniquely. The whole displacement component field can thus be reconstructed section by section from all lines of the micrograph that are parallel to the projection of the constant direction.

The following corollaries are immediate.

(i) *The vector displacement field can be reconstructed from three micrographs taken with non-coplanar diffracting vectors.*

(ii) *Three micrographs taken with non-coplanar diffracting vectors uniquely identify a defect.*

(iii) *Bright field and dark field micrographs contain identical information; for either can be used for reconstruction and both can be calculated from the displacement field.*

(iv) *If two micrographs have identical intensity distributions then they have identical phase distributions since they come from identical displacement component fields.*

(v) *A blank micrograph can only be from a null displacement component field.*

The importance of assuming a well-behaved displacement field is illustrated by the last corollary. When displacement fields are considered which contain step discontinuities (stacking faults) then it is well known that this corollary is not true and in fact none of the corollaries nor the theorem are then true. The problems of reconstruction of such discontinuous displacement fields will be considered in a subsequent paper.

The emphasis in this paper has been on the uniqueness properties of computer-generated electron micrographs and it is obvious that some of the concepts involved may not be very suitable for a practical reconstruction, e.g. the double differentiation of an experimental $I(y)$ or the analytic continuation of a function past a singular point of the reconstruction. Although the chance of encountering an exact singular point is small, it will be seen from (8) and (9) that in the neighbourhood of a singular point the accuracy of determination of β' would be poor. However, there are two constraints on the displacement field which have not been made use of and which would give some check on the accuracy of a practical reconstruction. Firstly, it would usually be the case that the displacement field would be an *elastic* one and it would be known that there are no body forces. In this case the displacements must satisfy the elastic equations of equilibrium for zero body force. Secondly, for each picture line, the field can be reconstructed in two ways, y increasing and y decreasing, and these must agree. This is equivalent to a closure condition that the reconstruction, having started in undistorted crystal at, say, $y = -\infty$, must tend to undistorted crystal again at $y = +\infty$. This would also seem to imply that not all functions of y are possible image functions $I(y)$ or $J(y)$ but that these come from a restricted class.

The restriction that has been made to the consideration of a parallel-sided untilted object is not fundamental and reconstruction is possible for any object of known shape. Suppose that $z = f_t(y)$ and $z = f_b(y)$ are the equations defining the top and bottom surfaces of the object section. Then (4) is modified by replacing δy in the first matrix on the right-hand side by $\delta y\{1+f_b'(y)\}$ and in the third matrix by $\delta y\{1+f_t'(y)\}$ and also by taking account of the variation of normal absorption due to the changing thickness of the object. Passing to the limit $\delta y \to 0$ now gives a more complicated set of four differential equations for the elements of $\mathbf{P}$ and equations (8) and (9) will have more complicated equivalents, but the general procedure remains the same.

Finally we give a simple example of the non-uniqueness that becomes possible when there is a singular combination of t and w. Consider the case of zero anomalous absorption, so that $Q = \mathrm{i}$, and with $w = 0$. Then, considering the equations (1) with initial conditions $\phi_0 = 1$, $\phi_g = 0$, if $\phi_0(z)$ and $\phi_g(z)$ are the solutions for any function $\beta(z)$ then $\overset{*}{\phi}_0(z)$ and $-\overset{*}{\phi}_g(z)$ are the solutions for the function $-\beta(z)$, so that both bright and dark field images have identical intensities for any t. Thus, for example, two dislocations with Burgers vectors $+\boldsymbol{b}$ and $-\boldsymbol{b}$ would have identical images in either bright or dark field.

VII. References

HEAD, A. K. (1967).—*Aust. J. Phys.* **20**, 557.

HIRSCH, P. B., HOWIE, A., NICHOLSON, R. B., PASHLEY, D. W., and WHELAN, M. J. (1965).—"Electron Microscopy of Thin Crystals." (Butterworths: London.)

HOWIE, A., and WHELAN, M. J. (1961).—*Proc. R. Soc.* A **263**, 217.

HUMBLE, P. (1968).—*Aust. J. Phys.* **21**, 325.