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

II.* DISCONTINUOUS FIELDS AND MANY BEAMS

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Summary

It is shown that the theorem of Part I, namely, that there is a unique reversible connection between displacement fields and electron micrographs for the case of two-beam diffraction and analytic displacement fields, can be extended to many-beam diffraction conditions. The case of a systematic set of diffracting vectors is parallel to the two-beam case with a unique reversible connection between one component of the displacement field and one micrograph. In the general many-beam case there is a unique reversible connection between the vector displacement field and three micrographs.

If the class of displacement fields is widened to allow discontinuities (stacking faults) then reconstruction is still possible but it is not necessarily unique as each discontinuity introduces a finite number of crystallographically different possibilities. A number of these may be rejected by comparing reconstructions from opposite directions but it is not certain that only one, unique, reconstruction will remain, although this is frequently the case.

INTRODUCTION

In Part I of this series it was shown that there usually is a unique and reversible connection between the displacement field of a cystal defect and its image in the electron microscope in the case where the micrograph is taken under two-beam conditions and the displacement field is analytic and has a direction along which displacements are constant. These restrictions were appropriate for discussing the uniqueness of computer-generated micrographs of dislocations. In this paper we consider the effect of relaxing these restrictions in two ways. Firstly, we consider micrographs taken under n-beam diffraction conditions (rather than two-beam) which is of increasing importance with the introduction of megavolt electron microscopes and, secondly, we allow discontinuities in the displacement field so as to include the important case of stacking faults in crystals.

MANY-BEAM DIFFRACTION CONDITIONS

In this section we consider the generalization of the two-beam case of Part I to the case where n beams are excited. The same sequence of argument is followed as for the two-beam case.

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Howie and Whelan (1961) have shown that for a displacement field $\boldsymbol{R}$, image formation in the n-beam case is governed by the n differential equations

$$\mathrm{d}\boldsymbol{v}/\mathrm{d}z = 2\pi\mathrm{i}\{\mathbf{A}+(\beta_g')_{\mathrm{diag}}\}\boldsymbol{v}\,, \tag{1}$$

where the components of the column vector $\boldsymbol{v}$ represent the amplitudes of the n waves, $\mathbf{A}$ is an $n\times n$ constant matrix, and

$$\beta_g' = \mathrm{d}\{\boldsymbol{g}\,.\,\boldsymbol{R}(z)\}/\mathrm{d}z$$

for each of the n values of $\boldsymbol{g}$ that are excited. The equations (1) become the Part I equation (1) in the two-beam case.

If an $n\times n$ scattering matrix $\mathbf{P}$ is defined in the same way as (2) and (3) in Part I then an equation similar to (4) in that paper gives a relationship between $\mathbf{P}(y)$ and $\mathbf{P}(y+\delta y)$, the scattering matrices of two neighbouring columns in a longitudinal section of a displacement field of the type being considered, i.e. one that has a direction in which displacements are constant. For $\delta y\to 0$ this becomes a set of n^2 differential equations for the components of $\mathbf{P}$. These differential equations have the same form as the corresponding equations (5) in Part I in that they are first-order linear differential equations in the n^2 components of $\mathbf{P}$ and the coefficients are linear functions of the $\beta_g'(y)$ and $\beta_g'(y-t)$.

Now suppose that from an electron micrograph taken with any one of the n beams, a picture line (which is parallel to the projection of the constant direction) has been selected and the process of reconstruction, started at $y = -\infty$ in good crystal, is proceeding in the direction of increasing y. Then corresponding to (8) and (9) in Part I there is a relationship

$$I_g''(y) = K_0+\sum_g K_g\,\beta_g'(y) \tag{2}$$

connecting the experimental $I_g(y)$ and the unknown $\beta_g'(y)$, where the K's represent known quantities that have already been reconstructed.

The simplest n-beam case is when the diffracting vectors form a set of systematic reflections so that each $\boldsymbol{g}$ is a scalar multiple of a fundamental $\boldsymbol{G}$. Then the $\beta_g'(y)$ are multiples of $\beta_G'(y)$ and equation (2) becomes

$$I_g''(y) = K_0+K_G\,\beta_G'(y)\,, \tag{3}$$

which can be solved for the one unknown function β_G' (provided K_G is not zero, which would give a singular point) so enabling continuation of the reconstruction. Thus this case is exactly parallel to the two-beam case and the basic theorem and its corollaries are equally true for n systematic reflections with the generalization that each of the n beams carries the same information about the object. The discussion of singular points is also similar, in that a singular point during reconstruction does not matter if the displacement field is analytic but that, for a singular point at the start of reconstruction, uniqueness cannot be proved.

For the general n-beam case, suppose that (R_1, R_2, R_3) are the components of the displacement field $\boldsymbol{R}$ referred to orthogonal axes fixed in the object. Then equation (2) can be written

$$I_g''(y) = K_0+K_1\,R_1'(y)+K_2\,R_2'(y)+K_3\,R_3'(y)\,, \tag{4}$$

where, once again, the K's represent known quantities that have already been reconstructed. Now suppose that, from three different electron micrographs, reconstruction of the vector displacement field is proceeding simultaneously and synchronously. Then for each micrograph there is an equation like (4) referring to the unknown displacements at the same physical point on the bottom surface of the object. These three equations can be solved for the three unknown R_i' (provided the equations are not linearly dependent, which would give a singular point) so enabling continuation of the reconstruction. Thus in the general n-beam case the basic theorem that gives a direct connection between one micrograph and one component of the displacement field is not true. However, it is true that, for the type of displacement field considered, the vector displacement field can, in general, be reconstructed explicitly and uniquely from three independent micrographs and that three such micrographs uniquely identify a defect. The exception will be, as in the other cases, when a singular point occurs at the start of reconstruction in which case uniqueness cannot be proved.

Displacement Fields with Discontinuities

In Part I and in the previous section we have restricted consideration to displacement fields that were assumed to be differentiable and, in cases where a singular point was encountered during reconstruction, to be further restricted to be analytic. This was appropriate for the discussion of many crystal defects such as dislocations, lines of dilation, etc. but excluded the important case of fault planes, across which the displacement field has a discontinuous jump. In this section we examine the effect of such discontinuities on the reconstruction of displacement fields from electron micrographs. The analysis is once again restricted to those displacement fields for which there is a direction along which displacements are constant so that all fault planes must contain the constant direction, and hence the trace of each fault plane on a longitudinal section of the object will be in the constant direction. Within this limitation a large number of configurations of interest are included, not only single fault planes in an otherwise perfect crystal but all the cases of multiple fault planes with dislocations for which Humble (1968) and Morton and Clarebrough (1969) have shown computer-generated micrographs.

For simplicity we consider in detail the two-beam case and reconstruction from a bright field picture for y increasing. The process of reconstruction described in Part I will be applicable where the displacement field entering the lower surface or leaving the upper surface is continuous, but, at those values of y where a discontinuity enters or leaves, a modified procedure is necessary. The finite jump in various quantities at such a discontinuity will be indicated by Δ. Suppose that between y and $y+\delta y$ a fault with displacement jump $\Delta\boldsymbol{R}(y)$ enters the lower surface and a fault with displacement jump $\Delta\boldsymbol{R}(y-t)$ leaves the upper surface. Then the scattering matrices of the columns at y and $y+\delta y$ are connected by the relation

$$[P(y+\delta y)] = \begin{bmatrix} 1 & 0 \\ 0 & \exp\{2\pi i\Delta\beta(y)\} \end{bmatrix} [P(y)] \begin{bmatrix} 1 & 0 \\ 0 & \exp\{-2\pi i\Delta\beta(y-t)\} \end{bmatrix}, \tag{5}$$

where

$$\Delta\beta(y) = \boldsymbol{g}\,.\,\Delta\boldsymbol{R}(y) \qquad \text{and} \qquad \Delta\beta(y-t) = \boldsymbol{g}\,.\,\Delta\boldsymbol{R}(y-t),$$

and expanding (5) gives

$$P_{00}(y+\delta y) = P_{00}(y), \tag{6a}$$

$$P_{0g}(y+\delta y) = P_{0g}(y)\exp\{-2\pi \mathrm{i}\Delta\beta(y-t)\}, \tag{6b}$$

$$P_{g0}(y+\delta y) = P_{g0}(y)\exp\{2\pi \mathrm{i}\Delta\beta(y)\}, \tag{6c}$$

$$P_{gg}(y+\delta y) = P_{gg}(y)\exp\{2\pi \mathrm{i}\Delta\beta(y)-2\pi \mathrm{i}\Delta\beta(y-t)\} \tag{6d}$$

for the components of P.

From (6) it will be seen that there is no discontinuity in either the bright field intensity $I = P_{00}P^*_{00}$ or dark field intensity $J = P_{g0}P^*_{g0}$. However, there is a discontinuity in the intensity gradient and this is the characteristic signature of a fault plane meeting a surface of the object. In Part I it was shown that the intensity gradient is given by

$$I' = P_{00}\,Q^*(P^*_{g0}-P^*_{0g})+P^*_{00}\,Q(P_{g0}-P_{0g}), \tag{7}$$

so that

$$\begin{aligned}\Delta I' &= I'(y+\delta y) - I'(y)\\ &= Q P^*_{00}(y)P_{g0}(y)[\exp\{2\pi \mathrm{i}\Delta\beta(y)\}-1]+Q^*P_{00}(y)P^*_{g0}(y)[\exp\{-2\pi \mathrm{i}\Delta\beta(y)\}-1]\\ &\quad -Q P^*_{00}(y)P_{0g}(y)[\exp\{-2\pi \mathrm{i}\Delta\beta(y-t)\}-1]\\ &\quad -Q^*P_{00}(y)P^*_{0g}(y)[\exp\{2\pi \mathrm{i}\Delta\beta(y-t)\}-1].\end{aligned} \tag{8}$$

This expression has been written in terms of the $P(y)$ components since these will be known during a reconstruction proceeding in the direction of increasing y, but by using (6) it can equally well be expressed in terms of the $P(y+\delta y)$ components for use in the reverse direction of reconstruction. It will be seen that the first two terms of (8) give that part of $\Delta I'$ due to the fault $\Delta\beta(y)$ entering the lower surface and the last two terms that part due to the fault $\Delta\beta(y-t)$ leaving the upper surface; also if either $\Delta\beta$ is zero then the corresponding contribution to $\Delta I'$ is of course zero.

Equation (8) gives the connection between the experimental $\Delta I'$ and the unknown $\Delta\beta(y)$ which is necessary for the continuation of reconstruction, but unfortunately this connection is not unique. Equation (8) is a quadratic equation in $\exp\{2\pi \mathrm{i}\Delta\beta(y)\}$ so that there are two possible values for this quantity and each of these only determines the fractional part of $\Delta\beta(y)$. If (8) is written in real form it gives a sinusoidal relation between $\Delta I'$ and $\Delta\beta$ with two fundamental solutions for $\Delta\beta$ in the range 0–1 and to each of these any integer may be added. It is well known that the images of stacking faults depend only on the fractional part of $\Delta\beta$ and so it is not surprising that reconstruction cannot determine the integer part of $\Delta\beta$. The reconstruction can be continued knowing only the fractional part of $\Delta\beta$ but there remains the choice between the two fundamental solutions. In practice one could continue both reconstructions and then perform the reconstruction in the opposite direction, which will also give two possible reconstructions. The true displacement field would then be the solution that is common. It is of course possible that both solutions are common so that there really are two valid reconstructions and an example of this, corresponding to the example of non-uniqueness given in Part I, is that for zero anomalous absorption and at the exact Bragg condition ($w = 0$) an isolated fault plane $\Delta\beta$ has an image which is identical with that of an isolated fault plane $-\Delta\beta$. Another case of non-uniqueness is that these two fault planes, $\Delta\beta$ and $-\Delta\beta$, also have identical images when the specimen thickness t, measured in units of ξ_g/π, satisfies

$$t(1+w^2)^{\frac{1}{2}} = n\pi$$

for any integer n. On the other hand, when the anomalous absorption is nonzero then every isolated fault plane has a unique image, apart from the ever present indeterminacy of the integer part of $\Delta\beta$.

Reconstruction from a dark field micrograph is similar to the bright field case with

$$\begin{aligned}\Delta J' = {} & Q^* P_{00}^*(y) P_{g0}(y)[\exp\{2\pi i\Delta\beta(y)\}-1]+Q P_{00}(y) P_{g0}^*(y)[\exp\{-2\pi i\Delta\beta(y)\}-1] \\ & -Q^* P_{gg}^*(y) P_{g0}(y)[\exp\{2\pi i\Delta\beta(y-t)\}-1] \\ & -Q P_{gg}(y) P_{g0}^*(y)[\exp\{-2\pi i\Delta\beta(y-t)\}-1] \qquad (9)\end{aligned}$$

in place of equation (8).

The preceding analysis of discontinuous displacement fields for the two-beam case can be generalized to n beams in the same way as the extension for continuous fields. Corresponding to (8) there is a relation

$$\Delta I_g' = K_0 + \sum_g [K_g \exp\{2\pi i\Delta\beta_g(y)\} + K_g^* \exp\{-2\pi i\Delta\beta_g(y)\}] \qquad (10)$$

connecting the jump in gradient of intensity of any one of the n beams with the unknown $\Delta\beta_g(y)$, where the K's represent known quantities that have already been reconstructed. If the n beams form a set of systematic reflections so that each $\boldsymbol{g}$ is a scalar multiple of a fundamental $\boldsymbol{G}$ then each $\Delta\beta_g(y)$ is a simple multiple of $\Delta\beta_G(y)$ so that (10) is a polynomial equation in the powers of one unknown, $\exp\{2\pi i\Delta\beta_G(y)\}$. This case is therefore parallel to the two-beam case except that this polynomial will have a greater multiplicity of possible fundamental solutions than the quadratic of the two-beam case. For the general n-beam case each $\Delta\beta_g(y)$ must be written in terms of the three components $(\Delta R_1, \Delta R_2, \Delta R_3)$ of the displacement field jump $\Delta\boldsymbol{R}$ and then (10) together with the two similar expressions for the other two reconstructions that are proceeding simultaneously give three multinomial equations to be solved for the three component jumps, with of course a multiplicity of solutions.

Although in all cases there are an infinite number of possible discontinuities that give the same jump in intensity gradient, there are only a finite number of physically different possibilities since a displacement jump of any lattice vector leaves a perfect crystal as a perfect crystal and any lattice vector can be added to a non-lattice vector discontinuity without changing the physical nature of the fault and without changing its image. The simplest case is the two-beam case with a low order diffracting vector, when there will be just two physical possibilities to be considered, and for practical reconstructions this is preferable to the greater number of possibilities that must be considered for high order diffracting vectors or many-beam excitation.

Discussion

The basic theorem of Part I exhibited two general properties of electron micrographs of analytic displacement fields for two-beam diffraction conditions, namely, that there is a unique relationship between micrograph and displacement field component, and that there is an explicit algorithm for reconstructing the displacement field in spite of the loss of all phase information. A proof of uniqueness is important not only for its own intrinsic interest but because it has been tacitly assumed when crystal defects have been identified by trial and error image matching. When trial and error fails, then the reconstruction algorithm offers another avenue for the identification of defects.

In this paper it has been shown that n-beam diffraction conditions also give these same properties of uniqueness and reconstructibility. However, the reconstruction algorithm is more complicated and without any compensating advantage, so that two-beam diffraction conditions are to be preferred.

For displacement fields with discontinuities it has been shown that there is a reconstruction algorithm but that nothing can be proved about uniqueness as there are multiple possibilities of reconstruction at each discontinuity. Once again two-beam diffraction conditions are preferable to n-beam conditions in giving the smallest number of possibilities. In any practical reconstruction the number of possibilities would probably be reduced by comparing reconstruction from opposite directions and may possibly leave a unique reconstruction. In fact the only known examples of non-uniqueness are for zero anomalous absorption, and attempts to construct two different displacement fields with identical images have been unsuccessful when the anomalous absorption is nonzero, except for the trivial case of faults that differ by a lattice vector. This suggests, but of course does not prove, that many reconstructions would lead to a unique result.

References

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