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May 1968

The differential equations of the two-beam dynamical theory of electron diffraction in an absorbing single crystal are, ignoring unimportant phase factors:[1]

$$\frac{dT(z)}{dz} = \frac{-\pi}{\xi_o'} T(z) + \left(\frac{i\pi}{t_o} - \frac{\pi}{\xi_g'}\right) S(z) \tag{1a}$$

$$\frac{dS(z)}{dz} = \left(\frac{i\pi}{t_o} - \frac{\pi}{\xi_g'}\right) T(z) + \left(\frac{-\pi}{\xi_o'} + 2\pi i S_g + 2\pi i \frac{d}{dz}(\vec{g}\cdot\vec{R})\right) S(z) \tag{1b}$$

where $T(z)$ and $S(z)$ are the transmitted and diffracted amplitudes, ξ_o' and ξ_g' the mean and anomalous absorption distances; t_o is the extinction distance, z the foil thickness, s_g the macroscopic deviation parameter, $\vec{g}$ the reciprocal lattice vector and $\vec{R}$ the displacement function of any defect present in the crystal. Occasionally, but not often, these equations can be handled by standard techniques; the wave vectors allowed in the crystal can be determined and the transmitted and diffracted waves expressed as linear combinations of waves with these wave vectors.

Numerical Method of Solution

In most cases the displacement function, $R(x,y,z)$, will be such that

the differential equations are not easily solvable. In such cases the differentials are approximated by $dF(z) \simeq \Delta F(z) = F(z+\Delta z) - F(z)$ and $dz \simeq \Delta z$. The differential equations then become:

$$T(z+\Delta z) = T(z)\left(1 - \frac{\pi \Delta z}{\xi_o'}\right) + S(z)\left(\frac{i\pi}{t_o} - \frac{\pi}{\xi_g'}\right)\Delta z \qquad (2a)$$

$$S(z+\Delta z) = T(z)\left(\frac{i\pi}{t_o} - \frac{\pi}{\xi_g'}\right)\Delta z + S(z)\left(1 - \frac{\pi \Delta z}{\xi_o'} + 2\pi i S_g \Delta z + 2\pi i \vec{g}\cdot\Delta\vec{R}\right) \qquad (2b)$$

where $\Delta\vec{R} = \vec{R}(x,y,z+\Delta z) - \vec{R}(x,y,z)$. These equations are then easily handled when the displacement function of a given defect is specified. Normally, a computer program is set up in which the value of Δz can be made quite small (units of a Burger's vector of hundredths of an extinction distance). Equation (2) specifies the incremental changes in the transmitted or diffracted amplitudes using incremental amounts of absorption and phase shifts, starting at the upper surface of the crystal where $T(0) = 1$ and $S(0) = 0$. Constant values of x and y are chosen and ΔR is used to determine the phase shift in the waves caused by the defect. These incremental phase changes, $2\pi i\vec{g}\cdot\Delta\vec{R}$, modify the phase shift of the perfect crystal, $2\pi i s_g \Delta z$, and hence change the diffracted intensities, relative to those from a perfect crystal, by a phase contrast mechanism.

The Column Approximation

The crystal is assumed to be composed of columns, each having an incident beam on its upper surface and transmitted and diffracted beams exiting from its lower surface. The width of such a column is then necessarily

dependent upon the diffraction angle and the foil thickness. The displacement function inside the column is assumed to vary only with z, and the deviation of the displacement function from that using average values of x and y is assumed insignificant. Therefore the column approximation becomes less accurate in thick foils, with higher order reflections and near the centers of defects. To obtain a two-dimensional image profile for a defect, Equation (2) is used on a series of parallel columns, the amplitudes at the bottoms of the columns converted to intensities and these plotted to give the profiles.

Point Defects

Assuming a spherically symmetrical displacement function, the displacement phase shift will be zero along a line through the defect normal to the reciprocal lattice vector. The phase shifts will have opposite senses on either side of the defect and the intensity profile for such a defect will have a line of no contrast through the center and quite often exhibit black-white contrast on either side of this line, depending on the foil thickness and the position of the defect in the foil.

Line Defects

Images of dislocations lying in the plane of the foil will be quite similar in cross-section to the profiles through the centers of point defects. However, diffraction conditions will vary according to the Burger's vectors of the dislocations, no strong images appearing when $\vec{g} \cdot \vec{b} = 0$. Special dislocation arrangements, such as small loops, dipoles and partial or superdislocations will modify the displacement functions and hence the details of the image intensity profiles.

Planar Defects

The incremental change in the displacement function, ΔR, is generally zero on either side of a planar defect and equal to some fraction of a lattice translation at the boundary. Stacking faults and antiphase boundaries inclined to the foil surfaces will normally exhibit fringes parallel to these surfaces since the amount of phase contrast present will vary with the depth of the defect in the crystal.

Volume Defects

When the transmitted and diffracted waves cross the boundary of a large region of material which has a different composition, orientation, or crystal structure, a new set of equations must be used which contain parameters (absorption and extinction distances, macroscopic deviation parameter and displacement function) suitable for the new region. The amplitudes of the waves at the boundary are calculated for the upper crystal and these are used as the incident amplitudes in the second crystal. There are usually phase changes associated with the boundary and perhaps even a dislocation structure at the boundary which must be considered in each crystal region. Overlapping crystal regions of similar composition and structure, such as twins and subgrains, will exhibit primarily a phase contrast mechanism. Precipitate contrast is generally achieved by means of an absorption contrast mechanism.

Special Consequences of Anomalous Absorption

In the presence of anomalous absorption, bright-field and dark-field images of a defect are no longer complimentary. The images will be similar

if the defect is in the top half of the crystal and pseudocomplimentary if the defect is in the lower half. Bright-field images of similar defects at the same distance above or below the center will be the same, hence dark-field images will be the opposite.[1] Defects near the surfaces will have anomalously wide images; the image widths can be used to estimate the displacements associated with point defect agglomerations and hence their sizes. The nature of a defect, whether vacancy or interstitial, can be determined from the anomalously wide images by observing the intensity variations about the center of the defect.[2] Defect positions can be roughly estimated and the slopes of defect planes and their character can also be determined.[3]

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