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Symmetry of Dislocation Images in Transmission Electron Microscopy

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The application of the reciprocity theorem in the field of electron diffraction has led to a number of useful relations between intensities of various diffracted electron beams [Pogany, A. P. & Turner, P. S. (1968). *Acta Cryst.* A**24**, 103]. Apart from perfect crystals, the theorem can also be applied to images of individual lattice defects, *e.g.* planar faults and dislocations [Howie, A. (1972). *Proc. Fifth European Congress Electron Microscopy*, Manchester, p. 408; Schapink, F. W. (1973) *Phys. Stat. Sol.* (*b*), **56**, K61]. The symmetry relations for dislocation images, both in bright field and dark field, are investigated in some detail. They may be divided into two groups: (i) Symmetry due to application of the reciprocity theorem, followed by a symmetry operation of the crystal associated with the diffraction vector (mirror inversion or central inversion). The relations found do not depend on the specific properties of the dislocation displacement field. (ii) Special relations due to symmetry properties of the displacement field, for particular dislocation geometries. The resulting symmetry depends on the degree of elastic anisotropy of the crystal.

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On Some Integral Aspects of the Dynamical Theory of Electron Diffraction

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As is well known, the dynamical theory of electron diffraction can be developed by using the basic statement of Bethe, H. [*Ann. Phys. Lpz.* (1928). **87**, 55] or integral treatments such as those of Fujiwara, K. [*J. Phys. Soc. Japan*, (1959), **14**, 1513], Kambe, K. [*Z. Naturforsch.* (1967), **22***a*, 422], Gjønnes, J. [*Z. Naturforsch*, (1972), **27***a*, 3] and Lannes, A. [*Phys. Stat. Sol.* (*b*), (1973), **56**, 513]. In a general way, the integral methods of approach seem preferable. Effectively, they are more general and more correct while at the same time facilitating mathematical and physical analysis of the diffusion problem. Some particular aspects of integral formalisms are of great interest in electron microscopy. In particular, integral methods allow us to introduce in a natural way the basic approximations of the dynamical theory of electron diffraction [Howie, A. & Basinski, Z. S. (1968). *Phil. Mag.* **17**, 1039; Lannes (1973); Gjønnes (1972)] (Forward diffusion approximation – Second, first and zeroth order approximation – Kinematical approximation). As an example, starting from the basic expressions of forward and backward diffusion [*cf.* relation (23) of Lannes (1973)]

$$\hat{\varphi}_g^{\pm} \simeq [\hat{\beta}_g^{\pm} \otimes \delta_0(z) + i\pi \hat{t}_g]_z^{*} \left[\pm y(z) \frac{\exp(2i\pi k_g^{\pm} z)}{q_g} \right] \tag{1}$$

where

$$\hat{\beta}_g^{\pm} = \frac{\hat{\varphi}_g'(\chi,0)}{4i\pi} - \tfrac{1}{2} k_g^{\mp} \hat{\varphi}_g(\chi,0)\,, \quad t_g = \alpha \sum_k v_{g-h} \varphi_h \tag{2}$$

$$k_g^{\pm} = -k_g \pm q_g\,, \quad q_g^2 = k_g^2 + \varepsilon_g^2 - w_g^2(\chi)\,, \quad \varepsilon_g^2 = K_0^2 - K_g^2\,, \tag{3}$$

and neglecting the term of backward diffusion as well as w_g^z, one obtains the integral expressions relative to the column approximation (zeroth order approximation)

$$\varphi_g = \left[\varphi_g^0 \otimes \delta_0 + i \frac{\pi}{k_g} t_g \right] \overset{*}{_z} Q_g \quad \text{where} \quad Q_g = y(z) \exp 2i\pi t_g^{+} z) \tag{4}$$

or alternatively

$$\varphi_g(\mathbf{r},z) = [\exp(2i\pi\tau_g^{+} z)] \left[y(z)\varphi_g^0 + i \frac{\pi}{k_g} \cdot \int_0^{l} t_g(\mathbf{r},\zeta) \exp(-2i\pi\tau_g^{+}\zeta) d\zeta \right] \tag{5}$$

where τ_g^+ is the excitation error $(\varepsilon_g^2/2k_g)$. In the derivation of (4) or (5), φ_g' has been neglected against $k_g\varphi_g$. The differential formalism may be obtained by deriving the convolution product (4) with respect to z. In this way, the differential formalism of Howie and Whelan can be regarded as the convolution inverse of the corresponding integral formalism. Effectively, writing $Q_g^{(-1)*}$ for the convolution inverse of Q_g,

$$Q_g^{(-1)*}=\delta_0'(z)-2i\pi\tau_g^+\delta_0(z)\,, \tag{6}$$

one obtains from (4)

$$\varphi_g'=\varphi_g^0\otimes\delta_0+i\frac{\pi}{k_g}[t_g-2k_g\tau_g^+\varphi_g]\,. \tag{7}$$

The standard form of Howie and Whelan [Whelan, M. J. (1970). *Modern Diffraction and Imaging Techniques in Material Science*, 35. Amsterdam: North-Holland; Lannes (1973)] can be obtained from (7) by proceeding to the change of variables

$$a_g=[\exp(2i\pi\mu_g)]\varphi_g \quad \text{where} \quad \mu_g=\mathbf{g}\,.\,\mathbf{W}\,. \tag{8}$$

With the kinematical approximation [Gevers, R. (1970). *Modern Diffraction and Imaging Techniques in Material Science*. I. Amsterdam: North-Holland] one gets the corresponding expressions of φ_g from (4) or (5) by performing the perturbation approach

$$t_g\simeq y\propto v_g\varphi_0\simeq y\propto v_g\varphi_0^0\,. \tag{9}$$

Effectively, taking into account (5), (9) and the change of variables (8), a_g can be written according to the kinematical expressions

$$a_g=[\exp 2i\pi(\tau_g^+z+\mu_g)]\,[y(z)\varphi_g^0+i\frac{\pi}{\zeta_g}\exp(i\theta_g\varphi_0^0\int_0^z\exp[-2i\pi(\tau_g^+\zeta+\mu_g)]\mathrm{d}\zeta]\,. \tag{10}$$

As can easily be shown from (4), (7) or (10), the distribution theory allows a convenient description of the boundary conditions.

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Calculated Images of Crystal Lattices by Axial Illumination with 1 MeV Electrons

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N-beam (001) electron-microscope lattice images (N=3,5,9) are calculated for gold when 1 MeV electrons and axial illumination are used. Conditions for obtaining images showing no artificial periodicity are determined. It is shown that in a particular range of thickness (40–60 Å or 140–160 Å) and with the proper defocusing distance high-contrast images would be obtained: the exact projected atomic positions are directly visible on these images. The influence of departure from exact symmetry conditions, and of large variation of the lattice parameter, are also studied. These calculations suggest that it would be possible to observe direct lattice images of metals and to study their defects with actual 1 MeV electron microscopes.