Proc. Fifth European Congress on Electron Microscopy, 1972

TOWARDS A MANAGEABLE THEORY FOR CROSS-GRATING HEED

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Under cross-grating conditions only a plane of reciprocal lattice points with vectors G contributes significantly to the observed diffraction. Thus the electrons move in an effective two-dimensionally-varying 'projected' potential $U(\underline{R})$, with Fourier coefficients $U_{\underline{G}}$ (Berry 1971 - hereafter called I). The vector $\underline{R}$ (=R, ϕ) lies in real space in the plane $\underline{G}$. Diffraction contrast arises from the beating of the different Bloch waves $b_j(\underline{r})$ as the specimen thickness z varies, the periodicities depending on the eigenvalues s_j, defined by

$$b_j(\underline{r}) = \tau_j(\underline{R}) \exp(-i s_j z/2k) \tag{1}$$

($\underline{k}$ is the wave vector of the incident beam).

In conventional many-wave theory (Howie 1970), the condition for s_j arises from a Fourier analysis of $\tau_j(\underline{R})$, which leads to the following determinantal equation over the set of $\underline{G}$'s:

$$\det_{\underline{G}\underline{G}'} \left\| \left[s-(\underline{K}_o + \underline{G})^2 \right] \delta_{\underline{G}\underline{G}'} - U_{\underline{G}-\underline{G}'} \right\| = 0 \tag{2}$$

($\underline{K}_o$ is the component of $\underline{k}$ in the plane $\underline{G}$, so that the angle of incidence θ is $|\underline{K}_o| / |\underline{k}|$). This procedure, which works well for the systematic case, runs into difficulties for cross-grating situations involving high energies and heavy atoms, because very large matrices arise.

We avoid this problem by using the KKR method of band-structure theory (Ziman 1971) in two dimensions, in which $\tau_j(\underline{R})$ is expanded within a single cell in angular momentum components $\tau_j^l(R) \exp(il\phi)$. Instead of (2), the condition for s_j is

$$\det_{ll'} \left\| (\cot \eta_l(s) - i) \delta_{ll'} + B_{l-l'}(s, \underline{K}_o) \right\| = 0, \tag{3}$$

where $\eta_l(s)$ is the l-wave phase shift for scattering from $U(\underline{R})$ (assumed to be a cylindrically symmetrical potential well within a single cell) at 'energy's, while $B_{l-l'}$ is a 'structure constant', defined in terms of the lattice sites $\underline{R}_j$ by

$$B_m(s, \underline{K}_o) = \sum_{i \neq o} \exp(i\underline{K}_o \cdot \underline{R}_i + im\phi_{\underline{R}_i}) H_m^{(1)}(\sqrt{s}\, R_i), \tag{4}$$

$H_m^{(1)}$ being the Hankel function of the first kind.

This formalism brings out the separation between 'bound' ($s_j < 0$) and 'free' ($s_j > 0$) bands, which is known (I, p708) to simplify analysis of the systematic case. The bound bands, where B_m is very small, are centred on the energy levels of U(R), for which

$$\cot \eta_l(s) = i, \quad \text{i.e.} \quad \eta_l(s) \longrightarrow -i\infty \;; \tag{5}$$

these bands correspond to almost flat branches of the dispersion surface. The nearly-free bands associated with each $\underline{G}$ - value satisfy

$$s = (\underline{G} + \underline{K}_o)^2 - \frac{4}{a^2} \sum_l \tan \eta_l (| \underline{G} + \underline{K}_o |^2), \tag{6}$$

where a is the lattice spacing.

As in the systematic case, we expect the bound bands to dominate the observed diffraction (I, fig. 10ff). The total number of these is n, roughly given by

$$n = \int_0^\infty R \, | U(R) | \, dR/4, \tag{7}$$

which are distributed over the angular momenta 0 to l_{max}, say. For $l > l_{max}$ there are no bound states and the η_l are negligible, even for $s > 0$. Thus the matrix in our eq. (3) has about l_{max}^2 important elements, while the usual eq. (2) has at least n^2 important elements (many more are often required to ensure convergence). Now, n greatly exceeds l_{max}, so that (3) is likely to be more useful in practice. As a numerical example, for Tungsten at 750kV, n is 18 while l_{max} is only 5.

References

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