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TRANSITION FROM QUANTUM TO CLASSICAL THEORY FOR HEED.

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As electron microscopes are used at higher and higher voltages, the associated computations based on the many-wave theory become more and more time-consuming and difficult to interpret. We have reformulated the theory enabling a sequence of new approximations to be derived, each becoming appropriate in a different energy range, and culminating, at the very highest energies, in the purely classical description. A detailed account of this new approach has been published elsewhere (Berry 1971). Here we shall just outline the methods used, and the principal conclusions.

In mathematical terms, it is necessary to solve the Schrödinger equation

$$\nabla^2\psi(\underline{r}) + (k^2 - U(\underline{r}))\psi(\underline{r}) = 0$$

for the wave function $\psi(\underline{r})$, where the relativistic energy k^2 and the reduced lattice potential $U(\underline{r})$ both depend on the bombarding energy E. We do not treat inelastic effects - of course they do occur, but it is not at all obvious (and probably wrong) to assume that at high energies they can be dealt with by suitably choosing an imaginary part to $U(\underline{r})$; work currently in progress is aimed at discovering just what form the correct high-energy theory of inelastic effects should take.

Above about 100 KeV the deflection angles θ of electrons transmitted through metal foils is small; more precisely, the condition

$$kt\theta^4/8 \ll 1$$

is valid for all energies and foil thicknesses t used or contemplated at present. Under these circumstances standard diffraction-theoretical methods applied to Schrödinger's equation yield a modified equation, in which the potential $U(\underline{r})$ is replaced by $\overline{U}(\underline{r})$, which is the average of $U(\underline{r})$ along the direction of the incident beam. [Under the stronger condition

$$kt\theta^2/2 \ll 1$$

which is valid only for very thin foils, the same methods yield the well-known phase grating approximation (Cowley & Moodie 1962) .] Depending on crystal orientation, $\overline{U}(\underline{r})$ can be one-dimensional (the case of systematic reflections) or two dimensional (the cross-grating case). The modified Schrodinger equation can be manipulated to yield the form of dynamical theory commonly used in HEED calculations (Howie & Whelan 1961).

Our detailed calculations have only been made for the case of systematic reflections, but a theory of the cross-grating case is nearly complete, and corresponding calculations will soon be performed. A cornerstone of our method is the formulation of dynamical theory in terms of the real-space potential $U(\underline{r})$ itself, rather than its reciprocal-space components U_g. The advantage of this approach is that standard methods of semiclassical analysis (e. g. the WKB method) can be used to yield the following testable information about the Bloch waves, valid for all cases except those to which the kinematic and two-beam theory applies:

1. <u>The Bloch eigenvalues s_j</u>. These are given by the solutions of

$$\cos\left[\operatorname{Re}\int_{\substack{\text{unit}\\\text{cell}}} dx\,(s_j-\bar{U}(x))^{1/2}\right]=\left[1+\exp\left\{2\operatorname{Im}\int_{\text{unit cell}} dx\,(s_j-\bar{U}(x))^{1/2}\right\}\right]^{-1/2}\cos(ka\theta_0),$$

where a is the spacing of the diffracting planes and θ_0 is the angle of the incident beam measured from these planes. These eigenvalues are reversed in sign relative to those conventionally used in dynamical theory, and are measured relative to the tops of the potential barriers between the atomic planes as zero, rather than from the mean value of $\bar{U}$ (x). This has the advantage of making our s_j values easily interpretable as 'energies' in a one-dimensional barrier penetration problem, so that if $s_j > o$ we have a 'free' state, and $s_j < o$ corresponds to a bound state. The square root factor on the right-hand side of our equation for s_j is just the WKB transmission coefficient for the barriers between planes, varying rapidly from o to 1 as s increases through zero.

2. <u>The number of contributing Bloch waves.</u> This depends on the energy, the angle of incidence, and the order of diffracted beam being calculated. For the bright-field case (zero-order beam) at normal incidence, the number of contributing beams is

$$\frac{1}{2\pi}\int_{\text{cell}}(-\bar{U}(x))^{1/2}\,dx$$

(The arbitrary zero of $\bar{U}(x)$ is chosen to lie halfway between the atomic planes.) This quantity increases with energy because of the relativistic E-dependence of U ($\underline{r}$).

3. <u>The number of diffracted beams appearing.</u> This depends on energy and angle of incidence. For normal incidence, we expect to see

$$\frac{a}{\pi}(-\bar{U}(a/2))^{1/2}+1$$

diffracted beams, a result that also follows from the classical mechanics of the electron propagation. ($\bar{U}$ (a/2) is the (finite) value of $\bar{U}$ (x) actually on the plane of atomic centres.)

4. <u>The critical angle.</u> When the angle of incidence θ_c exceeds the critical angle θ_c , equal to

$$(-\bar{U}(a/2))^{1/2}/k$$

all diffracted beams suddenly vanish whose order is such that their angle of emergence θ is negative. Thus selective Bragg reflection cannot occur if $\theta_0 > \theta_c$. The same part of the theory also gives a formula which predicts the range of angles of incidence for which any particular diffracted beam will exist.

The final part of the theory concerns those cases where E is so large that too many beams contribute for the Bloch-wave series to be of practical use. A simple transformation then produces a different series, whose terms represent the contributions to the diffracted beam emerging at angle θ from all the topologically different <u>classical</u> paths of particles incident at θ_0 and emerging at θ . This case is not yet realised experimentally for HEED, but it provides the appropriate description of heavy-particle channelling experiments.

References

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