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DISCUSSION

L. STURKEY: It would be interesting to compare exact calculations with the values obtained by Fujimoto's approximation process. Therefore, I suggest that several calculations be made by various people using their various systems and that comparisons be made with the exact result and Fujimoto's results. I will volunteer (if no one else does) to make the exact calculations be evaluating the complete scattering matrix.

Remark on the Diffracting Power of Net Planes with Very Large Spacing

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The approximative procedures in the theories of electron diffraction may generally be regarded as expansions with respect to reciprocal powers of the interaction constant $h^2/2m=150\text{eV}\cdot\text{Å}^2$. Considerations of some problems of recent interest, indicate that the ratio $s_h=\Phi_h\cdot d_h^2/(150\text{V}\,\text{Å}^2)$ plays an important role in determining the type of diffraction pattern to be expected from a space lattice, and in deciding for a suitable method of treating a problem. In this quantity which might be called "diffraction power of lattice planes h," d_h is the plane spacing of order h, and Φ_h is the Fourier coefficient of inner potential related to that order. In unit cells containing only a few atoms, which are mostly studied by diffraction, the spacing d_h remains always smaller than a few angstroms, and s_h rarely approaches the value 1. However, in the large cells of the complicated lattices characteristic of many organic compounds and silicates, and in crystals with superlattice structures, the spacing d_h can be rather large. Although Φ_h is then known to be very small, it can seldom be calculated because only a few lattice structures with large cells have been thoroughly investigated. A table given by Ibers[2] provides scattering powers of atoms at very small values of $2\cdot\sin(\theta/2)/\lambda=1/d_h$, and although tedious, the calculation of Φ_h is possible for known structures. Some structures of interest in the biochemical applications of electron microscopy are fatty acids with a large number of C atoms per molecule, and their derivatives. For the known structure of lauric acid (Vand, Morley and Lomer[2], $d_{001}=27.4$ Å), as an example, values of s_{00n} have been calculated. In the following table the values larger than 0.01 are given. The large value of s_{001} suggests that diffractions of several higher orders always occur simultaneously with (001). They must contribute significantly to the diffraction pattern, as well as to the fringe contrast in an electron micrograph. The range of incident angle

Table

n	s_{00n}
1	3.60
2	0.22
3	0.44
4	−0.074
5	0.062
6	−0.014
....	....
10	−0.018
12	−0.021
14	0.020

which gives the Bragg reflection (001), covers several (00*n*) Bragg directions, and the patterns will be fairly independent of the angle of incidence. This type of diffraction, perhaps, could explain the fact that electron micrographs of fatty acids and similar substances sometimes show good contrast of the fringes due to (001) planes when the object thickness is assumed to be sufficiently large, even though the heaviest atoms present are C and O.

The author is indebted to Miss Christa Lowack who has carried out the major part of calculations.

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The Dynamic Potentials in Electron Diffraction

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The dynamic potentials used in the two beam theory of electron diffraction are re-derived by using the integral equation rather than the fundamental equations. It is thereby ensured that the weak beams also satisfy the boundary conditions. The dynamic potentials thus obtained differ from the previously derived expressions in being complex and dependent on the size and shape of the crystal. When the product of wavelength and thickness goes to zero, convergence to the kinematic results is obtained.

1. Introduction

In the two-beam treatment of the dynamic theory in electron diffraction (see e.g. Pinsker[1]) the effect of the weak beams is taken into account by real increments to the Fourier coefficients of the potential:

$$\Delta U_{\alpha\beta}=\sum_{g}{}'' U_{g-\beta}U_{\alpha-g}/(k_g^2-k^2),$$
$$\alpha=0,h,\quad \beta=0,h, \tag{1}$$

where the summation is over all weak beams, i.e. excluding the strong beams, *0* and *h*, $\boldsymbol{k}_g=\boldsymbol{k}_o+2\pi\boldsymbol{g}$ is the wave vector inside the crystal of the weak beam *g*, and *k* is the length of the wave vector in vacuum. The potential expression including these terms is usually called the dynamic potential. It has recently been pointed out by Miyake[2] that the two-beam theory with dynamic potentials does not converge to the kinemaeic theory when the product of wavelength and crystal thickness λH, goes to zero.

It is the purpose of the present paper to point out, that if attention is paid to the boundary conditions on deriving the ΔU's, these will in general become complex and dependent on the size and shape of the crystal. The ΔU's thus obtained can then be shown to vanish in the limit of thin crystals or short wavelength and convergence of of the two beam result to the kinematic expression is obtained.

2. derivation of the dynamic potentials

Let us write the solution, of the Schrödinger equation inside the crystal, in the form:

$$\Phi(\boldsymbol{r})=\psi_0\exp(i\boldsymbol{k}_0\boldsymbol{r})+\psi_h\exp(i\boldsymbol{k}_h\boldsymbol{r})+\Delta\Phi, \tag{2}$$

where $\boldsymbol{k}_o$ and $\boldsymbol{k}_h$ are wave vectors of the direct and the strong reflected beam respectively.

The essential idea in the introduction of dynamic potentials is that the weak beams, $\Delta\Phi$, can be expressed in terms of the ampli-

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