Proc. Fifth European Congress on Electron Microscopy, 1972

# SEMICLASSICAL PREDICTION OF INCREASED PENETRATION NEAR CERTAIN VOLTAGES

P A Doyle and M V Berry

H H Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

A major advantage of high voltage microscopes is the improved electron penetration achieved. This paper suggests that the penetration may be maximized in specific voltage ranges characteristic of the specimen, rather than simply at the highest voltage available.

Radi (1968) showed that when the inelastic scattering processes are highly localized, their effect on the elastic beams could be included by writing the lattice potential in the systematics case as $U(x)+iU^{i}(x)$. By extending the treatment of elastic scattering given by Berry (1971), we have found that for this localized approximation, the wave function $\psi(x,z)$ of the electron at depth z in a crystal is

$$\psi(x,z)=\sum_j C_j \mathcal{T}_j(x)\exp\left[i(s_j+is_j^{i})/2k\right]\exp(iK_o^2 z/2k)\exp(ikz) \tag{1}$$

where $K_o/k$ is the angle of incidence. First order perturbation theory gives an expression for the imaginary part $s_j^{i}$ of the energy level j. Using WKB approximations for the Bloch eigenfunctions $\mathcal{T}_j(x)$ (see Berry 1971, eqns. 67 and 69), we find that

$$s_j^{i} = \int_o^{a/2} \frac{U^{i}(x)dx}{\left[s_j-U(x)\right]^{\frac{1}{2}}} \Big/ \int_o^{a/2} \frac{dx}{\left[s_j-U(x)\right]^{\frac{1}{2}}} \tag{2}$$

where a is the lattice spacing. Approximate parabolic fits to the more accurate values of $U(x)$ and $U^{i}(x)$ suggested by Steeds (1970) are used to simplify preliminary calculations. These give the correct form near x=0 (the top of the potential barrier), which is most important for the present work.

Fig. 1 shows $s^{i}$ against s for gold (111) systematics at 600 KV. For a particular orientation defined by $K_o$, only a discrete set of real eigenvalues exists. The low values of $|s^{i}|$ near s=0 (corresponding to 'Bloch wave channelling' between atomic planes) can be used to maximize penetration at an accelerating voltage E provided that

(A) a state exists at or close to s=0 for some $K_o$, and

(B) this state is strongly excited.

For a state to exist at s=0 we can show (Berry 1971, eqs. 49, 65) that

$$\cos\Phi = (1/\sqrt{2}).\ \cos(K_o a) \tag{3}$$

where $\Phi = (m/m_o)^{1/2}.(a/2)\cdot\left|U(a/2)_{E=0}\right|^{1/2}$. Fig. 2 shows $\cos\Phi$ for incident electron energies up to 4 MeV. Clearly, there are energy bands for which a value of $K_o$ satisfies eqn. (3). Within these bands, the condition (A) above is satisfied.

The values of $K_o$ at which a state $s_j=0$ exists in the lowest complete energy band are shown on Fig. 3. These values repeat every $2\pi/a$. From Berry (1971, eqns. 88), it follows that the contribution from a state j to the diffracted beam G is principally determined by $f(s_j, K_o, K_G)$, where $K_G=K_o+G$, and

$$f(s,K_o,K_G) = 1 \Big/ \left[(K_o^2 - s)(K_G^2 - s)\right]^{1/4} \ln\left(4\,|U(a/2)| \big/ |s|\right) \qquad (4)$$

This function is shown for low values of s on Fig. 4 for the bright field (G=o) taking $K_o^2 = 0$ and 0.5. Clearly, a state $s_i = 0$ contributes most strongly to the bright field if it is excited when $K_o = 0$. From Fig. 3, this occurs only at 800 KV, i.e. when $\cos \Phi = +1/\sqrt{2}$. Thus exceptionally strong anomalous transmission for bright field occurs at 800 KV, and also from Fig. 2 at 300 and 3,140 KV. Also, for all $G \neq 0$, f (eqn. (4)) still diverges so that the other beams are also quite well transmitted. Therefore, high contrast as well as high intensity are expected in bright field for normal incidence at these voltages.

The maximum penetration may in fact be achieved when a state $s_i$ slightly greater than zero is excited by $K_o = s_i^{1/2}$, since such a state would contribute more strongly as on Fig. 4. When $\cos \Phi = -1/\sqrt{2}$ on Fig. 2, good transmission is possible for only one diffracted beam, giving no gain in contrast. While the actual voltages predicted here may not be accurate, it appears that exceptionally good bright field contrast from thick specimens may be observed near normal incidence within quite narrow voltage ranges. Preliminary calculations suggest that these ranges may be about 100 KV wide for gold. When the voltage is increased past such a range, contrast decreases.

P A Doyle is indebted to the S. R. C. for financial support.

References

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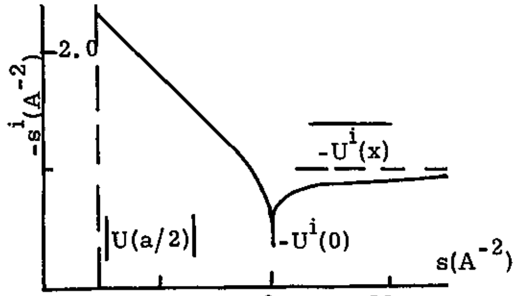

Fig. 1.

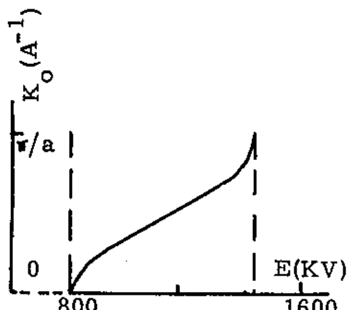

Fig. 3.

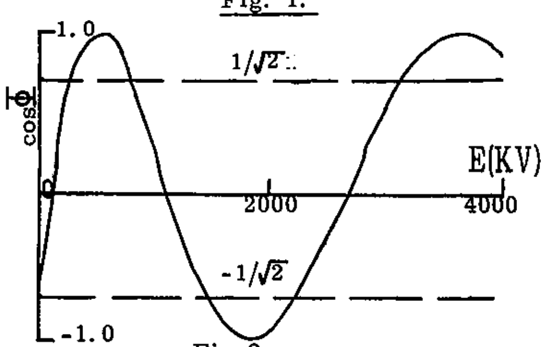

Fig. 2.

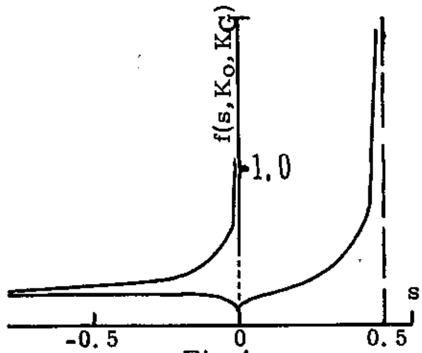

Fig. 4.