A NEW INTERPRETATION OF BEND CONTOURS IN TERMS OF SEMICLASSICAL MECHANICS

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Exact Bloch wave calculations of the bend contour intensity $|A_G|^2$ for the $m$th diffracted beam are fairly easy (Steed 1970) in many-beam cases, but these do not lead to a transparent qualitative picture of the origin of the shape of the contours as a function of thickness $z$ and direction of incidence $K_o$.

We propose an alternative explanation of the bend contours, based on the classical paths of the electrons through the one-dimensionally periodic lattice potential $U(x)$ (fig. 1a) whose Fourier components $U_m$ constitute the initial data for Bloch wave calculations. According to the principles of semiclassical mechanics (Berry & Mount 1972) the amplitude $A_G(z, K_o)$ is approximately

$$A_G(z, K_o) = \sum_m \rho_m(z, K_o) \exp (iW_m(z, K_o)) \tag{1}$$

where $m$ labels the different possible classical paths for which electrons incident at $K_o$ emerge at $K_G$ after traversing a thickness $z$, $W_m$ is the phase along the $m$th path, and $\rho_m$ is the density along the path (which measures the divergence and focussing of a small bundle of paths). The analytical theory deriving (1) from the Bloch wave series may be found in sec. 5 of Berry 1971 (hereafter called 1). From eq. (1) we expect two main types of feature in the image plane $z, K$: (a) caustics, which are lines along which $\rho_m$ is infinite, corresponding to an envelope of the family of paths $m$ (as at the focus of a lens, or the light from a water-drop in a rainbow), (b) interference fringes, which are lines along which the phase difference $W_m - W_n$ is constant for two paths $m$ and $n$ which coexist in a region free from caustics (e.g. the set of hyperboloids locating Young's fringes from two coherent sources).

For the periodic potential of fig. 1a, the classical paths fall into two classes:

(i) **Quasi-free paths** (fig. 1b), where the electron may travel between cells by crossing the interatomic planes.

(ii) **Bound paths** (fig. 1c), where the electron winds back and forth within a single cell.

Both classes of paths may be further specified by an index $m$ corresponding to the number of crossings of atomic planes, as detailed in 1 (sec. 5, figs. 12-14). We have calculated $W_m$ and $\rho_m$ for the bright field in the case of a potential parabolic inside each cell of width $a$, with a maximum depth $U_{max}$ on the atomic planes. We find that the quasi-free path structure is dominated by a series of caustics for each $m$, resembling hyperbolas, satisfying the equation

$$K_o = \sqrt{\frac{U_{max}}{U_{max}} \cosh \left( \frac{z}{\sqrt{\frac{U_{max}}{kam}}} \right)} \quad m = 1, 2, \ldots \tag{2}$$

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where \( k \) is the wave number of the incident electrons. The bound paths have no caustics, and we expect to see interference fringes roughly parallel to the \( K_0 \)-axis out to the 'critical direction' \( K_0^c = \int U_{\text{max}} \) (I, eq. 75). The fringe spacing at \( K_0 = 0 \) is predicted to be

\[
\Delta z = \frac{4\pi k}{U_{\text{max}}}
\]

(3)

These bright-field bend contours predicted by semiclassical mechanics are sketched in fig. 2: They are obviously qualitatively similar to experimental and computer-simulated micrographs, and a preliminary comparison for Gold (600 KV (111) Steeds 1970, 650 KV (200) Richards & Steeds 1971) gives quantitative agreement within a factor 2. If more detailed analysis confirms these results, the way will be opened for new methods of understanding images of defects in many-beam situations, simply by calculating the classical paths in their neighbourhood.

References

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