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 G^{th} diffracted beam are fairly easy (Steeds 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_G 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

$$A_G(z,K_o) \approx \sum_m \sqrt{\rho_m(z,K_o)} \exp(iW_m(z,K_o)) \qquad (1)$$

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 ρ_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 I). From eq. (1) we expect two main types of feature in the image plane z, K_o: (a) caustics, which are lines along which ρ_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 I (sec. 5, figs. 12-14). We have calculated W_m and ρ_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 hyperbolae, satisfying the equation

$$K_o = \sqrt{U_{max}} \operatorname{cosech}\left(\frac{z\sqrt{U_{max}}}{kam}\right) \qquad m = 1, 2 \text{------} \qquad (2)$$

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_o-axis out to the 'critical direction' $K_o^c = \sqrt{U_{max}}$ (I, eq. 75). The fringe spacing at $K_o = 0$ is predicted to be

$$\Delta z = \frac{4\pi k}{U_{max}} \tag{3}$$

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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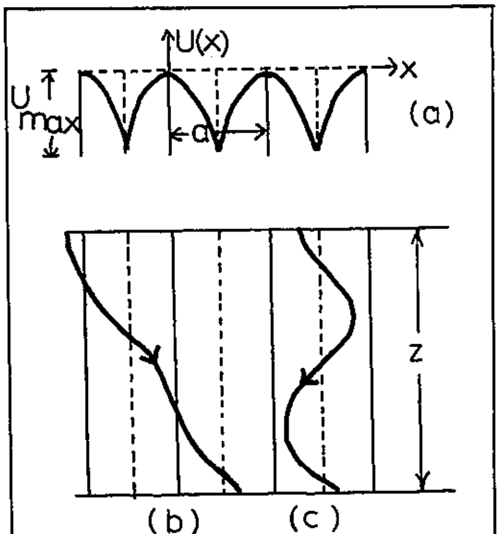

Fig1 (a) periodic potential
(b) quasifree path
(c) bound path

------- atomic planes

_______ interatomic planes

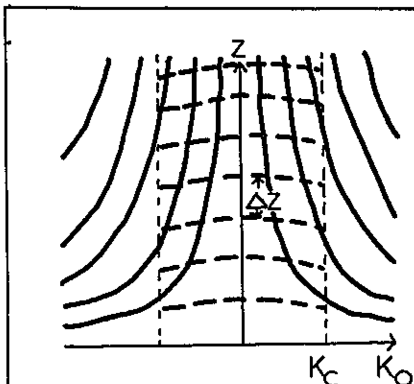

Fig2 semiclassical bright-field bend contours

------ interference fringes

_____ caustics