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Short Communications

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Acta Cryst. (1970) A**26**, 152

Comments on the BJR theory of electron diffraction.

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In the BJR theory of electron diffraction an absorption effect due to weak beams is introduced into the two-beam approximation for the dynamical diffraction of electrons by thick crystals. This is shown to be unjustified for diffraction from perfect crystals. The use of the theory to derive the temperature dependence of diffraction intensities must therefore be modified.

The BJR theory of electron diffraction (Boersch, Jeschke & Raith, 1964) has been used successfully as the basis for interpretation of intensity measurements in electron diffraction, particularly in relation to the temperature variation of relative intensities of rings from thick polycrystalline specimens (Glaeser & Niedrig, 1966; Albrecht & Niedrig, 1967, 1968). However, the basic assumptions of the theory have been brought into question (for example by Fukuhara, 1965) chiefly because of the introduction of an absorption effect due to weak beams in the two-beam approximation to the dynamical theory of electron diffraction. Starting from a slice-type formulation of scattering theory, the scattering from an individual layer of atoms is regarded as the scattering by a phase grating which can be expressed in terms of complex atomic scattering factors. This is somewhat similar in principle to the assumptions of the theory of Cowley & Moodie (1957) which has been quoted in this connexion. Hence we feel it is appropriate to discuss the differences between the Cowley–Moodie and the BJR theories and to point out the nature of the deficiency in the latter.

In the approach of Cowley & Moodie (1957) the transmission of an electron wave through a thin slice of crystal is treated in terms of a modification of the phase of an electron wave by a two-dimensional projected potential distribution, acting as a planar phase-grating, plus the modification of the phase due to Fresnel diffraction between slices. It has been shown (Moodie, 1968) that, in the limiting case of the slice thickness tending to zero, this gives a solution to the scattering problem which is exactly equivalent to a solution of the Schrödinger wave equation. In the absence of absorption due to inelastic scattering or elastic diffuse scattering by crystal imperfections, the periodic potential distribution inserted into the Cowley–Moodie formulation and into the wave equation is a real one.

For purposes of the calculation of intensities, the Cowley–Moodie formulation has been used with finite slices. In the case of a slice thickness corresponding to a single layer of atoms, which gives no appreciable error in calculated intensities, the scattering by the slice could be written approximately in terms of the complex atomic scattering amplitudes deduced by partial wave scattering theory by Ibers & Hoerni (1954) or Raith (1968), but this constitutes only a convenient mathematical device for representing the scattering from a real potential. In such scattering by a pure phase grating, energy is conserved and no absorption is involved.

In the BJR approach however, when the scattering by a single layer of atoms is expressed in terms of complex scattering amplitudes, manipulation of the expressions appears to lead to the introduction of an absorption effect which is mathematically equivalent to the use of a complex potential in the wave equation. This complex potential is formed by summing over complex atomic scattering amplitudes in the same way as the real potential is obtained by summing over the real, first Born approximation, scattering amplitudes which are used because they are proportional to the structure amplitudes obtained by Fourier inversion of the real atomic potential distributions. The origin of the absorption is said to be the effect of weak beams on the two strong beams considered in a two-beam approximation, since for each single-atom layer some intensity will be scattered into the weak beams. The error in this treatment arises from the fact that, while scattering from strong beams into weak beams is taken into account, the scattering from weak beams into strong beams is not.

Complete *n*-beam calculations, such as those of Goodman (1968), have clearly demonstrated that, for thickness greater than about one or two 'extinction distances' of the strong beam, a state of equilibrium is reached so that for all greater thicknesses the weak and strong beams have, on the average, the same relative intensities. This implies that the scattering from strong to weak beams is exactly matched by scattering from weak to strong beams. Thus the effect of weak beams is not that of an absorption except for very thin crystals. The main effect for thick crystals is to modify the effective structure factor for the main beams, giving changes in the average intensity and extinction distances. For rings or arcs from polycrystalline specimens, the changes may be small except in special cases such as for higher orders of strong inner reflexions (for a review, see Cowley, 1967).

The temperature dependence of diffraction rings given by polycrystalline specimens should be describable in terms of

(1) the Debye–Waller temperature factors in the structure factors for the strong reflexions,

(2) the absorption effects on the strong beams due to thermal diffuse scattering (Hall & Hirsch, 1965; Cowley & Pogany, 1968),

(3) the *n*-beam interactions between strong and weak beams, which should be strongly temperature dependent because they are affected by the Debye–Waller factors and absorption effects on all beams (Goodman, to be published),

(4) the temperature dependence, if any, of other absorption effects such as those due to plasmon or single electron excitations or scattering by crystal defects or disorder.

The fact that very good agreement has been found between the predictions of the BJR theory and experimental measurements on such a temperature dependence suggests that comparison with this type of experimental evidence may not be a very sensitive test of the rigour of an approach to dynamical theory, in that any theory taking dynamical effects into account to a sufficient degree may give much the same results.

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Acta Cryst. (1970). A**26**, 153

Interferometric study of liquid crystalline surfaces.

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The optical interferometric technique has been used to examine liquid crystalline surfaces. Topographs are given of stepped and faceted drops. Some new surface features of the smectic and cholesteric phases are also presented. The nematic phase gives fringe contours similar to those of the isotropic liquid.

We have used the optical interferometric technique to examine the topographical features of liquid crystalline surfaces. A tiny droplet of the specimen was taken on a microscope slide and a thin cover slip was placed over but not actually touching it. Two-beam interference fringes with monochromatic radiation (λ5893 Å) formed between the upper surface of the droplet and the lower surface of the cover slip were observed and photographed through a reflexion microscope provided with a hot stage (see, *e.g.* Tolansky, 1948). The substance was heated till it became liquid and then brought to the mesomorphic phase by slow cooling to any desired temperature. Under favourable conditions, an optically homogeneous drop could be formed. A few typical cases are described below.

Fig. 1(*a*) illustrates the fringe patterns obtained from a solution of potassium oleate in aqueous methyl alcohol. The solution exhibits lyotropic mesomorphism at room temperature. Microscopic examination (in transmitted light) of the textures of the mesophase showed that they are identical with those of potassium oleate in aqueous ethyl alcohol as reported by Chistyakov (1961), confirming that the phase is smectic. The fringe pattern in Fig. 1(*a*) reveals the characteristic stepped regions of the smectic phase, the origin of which can be explained from surface energy considerations (Chandrasekhar, 1966). Observations through a polarizing microscope between crossed polars showed that the specimen was optically homogeneous with the long axes of the molecules parallel to the direction of observation *i.e.* normal to the plane of the paper; in parallel light complete extinction was obtained for all settings of the microscope stage, and in convergent light the uniaxial cross was seen. Further, the interference colours produced by inserting a full-wave plate between the crossed polars established that the specimen was optically positive (see, *e.g.* Ennulat, 1968). Fig. 1(*b*) shows a stepped drop [goutte à gradins (Grandjean, 1917)] of the same substance.

Fig. 2 illustrates the striking changes in the topography of a large drop of a mixture of methyl stearate and methyl palmitate when cooled from the liquid to the liquid crystalline phase. In the latter phase the long axes of the molecules were parallel to the direction of observation. The smooth, rounded surface of the liquid drop [Fig. 2(*a*)] develops plane faces and sharp edges in the mesophase [Fig. 2(*b*)]. The faceted drop (goutte à facettes) was discovered by Bernal & Crowfoot (1933) in one of the mesophases of ethyl anisal *p*-aminocinnamate and of ethyl-phenyl benzylaminocinnamate. The presence of faces, edges and corners indicates a very high degree of molecular order resembling that in a crystalline solid, though as far as its mechanical properties are concerned this phase is more appropriately described as