Bragg Case in Laue Case Diffraction

A Maybe Novel Statement on Wave Field Beams

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Dedicated to Prof. Hildebrandt on the occasion of his 60th birthday

The boundaries of wave field beams in Laue case diffraction are in their function identical with crystal surfaces parallel to the lattice planes, reflecting in the symmetrical Bragg case. On extreme presumptions the wellknown Darwin-Ewald total reflection may occur.

A plane wave assumed to be diffracted by lattice planes normal to a crystal surface (symmetric Laue case) builds up inside the crystal four wave fields (Ewald waves), each of them being the result of the superposition of two waves, the continued primary wave and the diffracted one. If additionally the incident wave is assumed to be polarized, with the electric vector normal to the plane of incidence, the number of wave fields gets restricted to two, with directions of propagation (Poynting vectors, dashed in Fig. 1a), symmetrical to the lattice planes and perpendicular to the dispersion surface in the correlated tie points A_1' and A_2' (Fig. 1e, dashed arrows). These tie points for their part are defined by the exact direction of the external incident wave, marked by the "excitation point" P_L' on the "excitation surface". We now regard the special case of optimal diffraction (maximal intensity), P_L' having gone to the "Laue point" L and A_1', A_2' to A_1, A_2, so that both directions of propagation coincide in parallelity to the lattice planes. Then each of these parallel wave fields may be — and usually is — concieved otherwise, namely described as a product of a travelling and a stationary wave, the former one progressing parallel to the lattice planes with velocity $c \cdot \cos \vartheta$, the latter one having node and antinode planes parallel to them. Or in other words, a travelling wave modulated by a stationary one.

This aspect, as derived from the dynamic theory, not containing any "zick-zack" reflection between both single waves, has been displayed many years ago, e.g. by Borrmann [1]. Borrmann even goes as far to deny any further real existence of the single waves building a wave field ("keine Einzelwellen mehr", see [1], p. 112).

For the wave field A_1 the nodes, for A_2 the antinodes coincide with the planes of maximal electron density. Therefore the latter one undergoes increased, the former one decreased absorption (Borrmann effect), and in greater depth the field A_2 is filtered away, and only A_1 remains.

Now an extreme case may be assumed: "zero thickness" of the single lattice planes separated by the inter-lattice distance, for example the lattice being a point lattice as assumed in Ewalds early theory. Then the diameter of the dispersion hyperbola is increased to an amount that its outer vertex, together with A_1, coincides with the Laue point L (Figure 1f). The wave field then is no longer in any interaction with the crystal lattice, because all matter, the scattering and the absorbing one as well, is located in the node planes of the electric field strength. That means, the crystal lattice may be removed without any distortion of this wave field. The wave field propagates in an "optical empty" space. Its state is just that one of two crossing coherent waves, in light optics well familiar, e.g. in the case of specular reflection of one plane wave (stationary light waves, Wiener interferences).

All that is exactly true for the extreme special case exposed before. But qualitatively the same behaviour applies also to lattices with basis, i.e. lattice planes of finite "thickness", and besides for the wave field A_2. Only irrelevant modifications take place, concerning minute changes of the wave directions and the disappearing of the vertical intensity decrease of field A_2 if the scattering and absorbing matter is removed together with the removal of the lattice.

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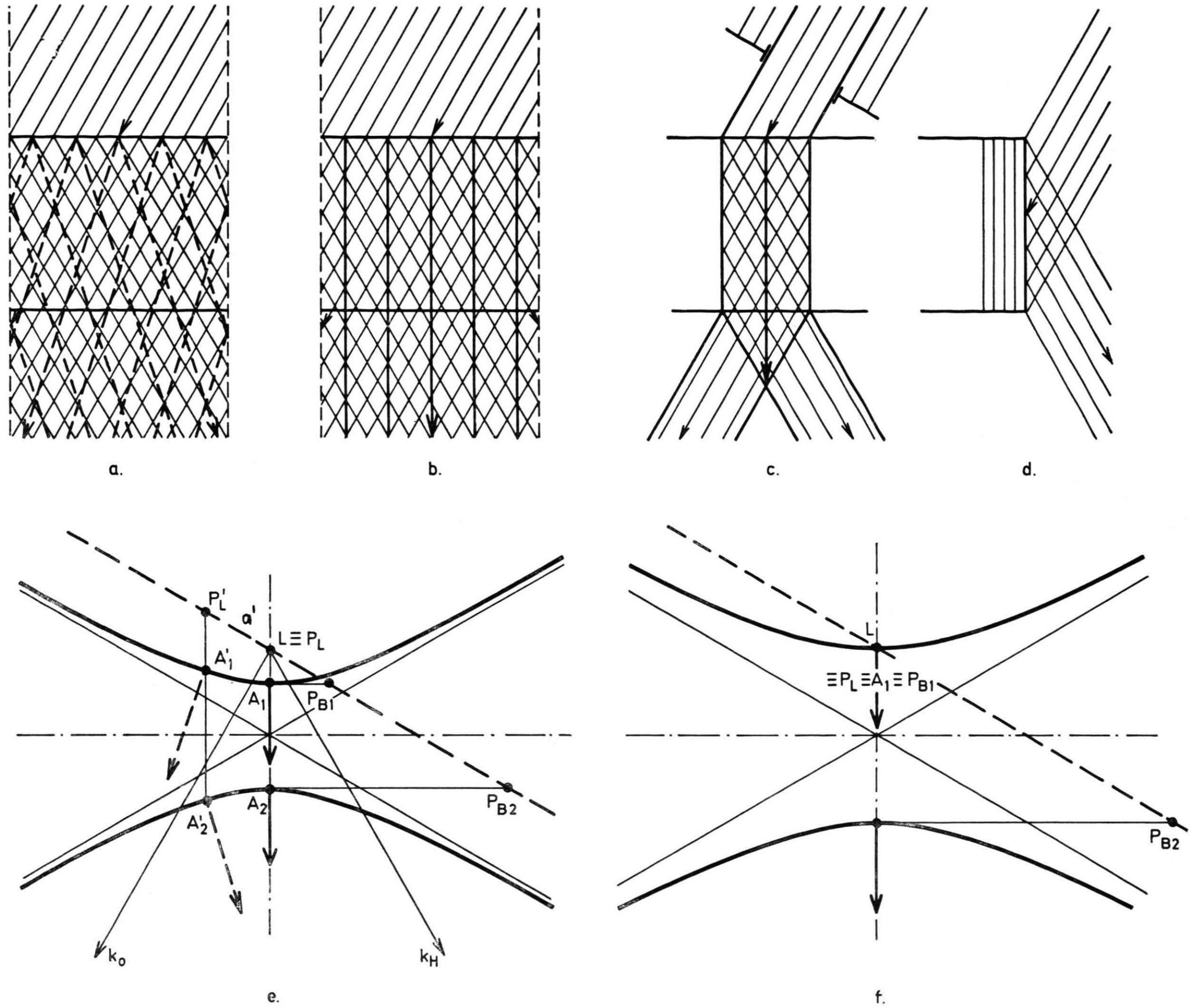

Fig. 1. Laue case and correlated Bragg case diffraction. a—d in the real, e and f in the reciprocal space, a and b, waves of infinite lateral extension, a, $\Delta\vartheta$ ($=a'/k_0$) finite (<0), corresponding tie points in e: A_1' and A_2', b, $\Delta\vartheta=0$, corresponding tie points A_1 and A_2,c, beam of finite cross section, d, corresponding normal Bragg case, e, Dispersion surface for lattice planes of finite thickness, f), Dispersion surface for lattice planes of zero thickness (point lattice).

So far waves of infinite lateral extension have been regarded. But now the question arises, why a *beam*, of finite cross section of such a wave field (Fig. 1c) travels straight down, parallel to the lattice planes. Why doesn't it spread sideways like beams of crossing plane waves, in spite of the fact that it progresses in an "empty" space? And nevertheless after having left the lower crystal surface, it gets split in the two beams R_0 and R_H! What is the role of the lattice preventing it from splitting earlier?

The explanation results from the fact that the wave fields *really* are superpositions (or Fourier components) of the two diffracted waves, R_0 and R_H, and that the formal aspect of them as of modulated waves progressing straight downward gives no hint for at an evident understanding.

Having a glance on the corpuscular aspect we see: The velocity of photons can't be smaller than c. Therefore a stream of photons, with velocity $c \cdot \cos\vartheta$, the velocity of the progressive wave, is not possible. Rather there are really *two* crossing streams of them inside the beam, and just as well *two* crossing waves too.

But then, evident for the waves as well as for the photons, how are they prevented from leaving the beam? The only acceptable conclusion demands that they are reflected by its "walls". This reflection may easily be explained by the fact that the "optical empty" space found by the wave field A_1 due to the concentration of the scattering matter in the node planes of the stationary wave is present *only inside the beam.* Outside there are no node planes, for there is no wave going inward. So for the component going outward the situation is quite that of a wave incident on the beam wall accurately representing a crystal surface which reflects it in the symmetrical Bragg case. The correlated tie points A_1 and A_2 for both wave fields would as well be excited by two waves from outside, if "outside" means the space inside the beam from which the lattice is thought to be removed. The exact primary directions of incident waves exciting these tie points would have to be marked by the excitation points P_{B1} and P_{B2}. They denote the limiting angles of the Darwin-Ewald range of total reflection. For one single primary direction, if the excitation points P_{B1} and P_L coincide with the tie point A_1 in L, the identity of the beam walls with crystal surfaces replacing them is quantitatively perfect for the wave field A_1.

But what has been explained before for the whole wave fields is true also concerning the functional identity of the beam walls with crystal surfaces. Qualitatively this identity is valid for any wave field beams, correlated to any tie points on any dispersion surface, i.e. for any kinds of lattices. And it should be emphasized once more that this Bragg case in Laue case reflection is not a mere "aspect" but a real statement.

[1] G. Borrmann, Z. Krist. **106**, 109 (1954).