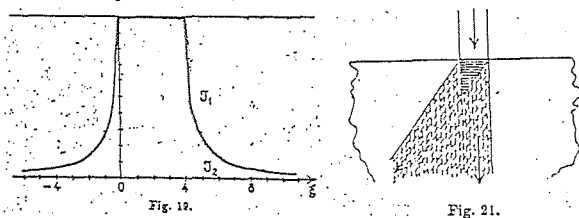


597. Teil IV: Aufstellung einer allgemeinen Dispersionsbedingung insbesondere für Röntgenfelder. *Z. Krist.*, 1937, 97, 1-27.

It is interesting to note that he himself worked out only on perfect crystals, although he often expressed to us his interests in imperfect crystals. The fact is probably due to his aesthetic attitude toward physical theory. It is true that his theory is much difficult compared with the contemporary theory of Darwin (1914) and those of Bethe (1928) and Laue (1931). This is inevitable because he was concerned with the foundation of optics covering all from visible rays to X-rays. Nevertheless, if we look at the drawings (below) and equations in the papers cited above, we can immediately see how enormously we owe him in fundamental concepts of crystal diffraction. This situation is not confined to the diffraction theory. The Ewald method of evaluating the lattice sum (F. Seitz: The modern theory of solids, 1940, p.77) and Ewald-Oseen theorem (M. Born and E. Wolf: The principles of optics, 1959, pp.99-100) are examples. The concept of Bloch wave was in fact originated by Ewald.



From Teil III cited above.

11.X-4 THE RECIPROCAL LATTICE IMBEDDED IN FOURIER SPACE. By D.W.J. Cruickshank, Chemistry Dept., UMIST, Manchester M60 1QD, England.

The reciprocal lattice and the sphere of radius  $K_0 (=2\pi/\lambda)$  were introduced by Ewald (*Phys. Z.*, 1913, 14, 465-472) directly from his dynamical theory of crystal optics, which examined the internal aspects of wave propagation in crystals. Laue extended Ewald's orthorhombic treatment to general triclinic lattices using Gibbs' reciprocal vectors. In 1921 (*Z. Krist.*, 56, 129-156) Ewald presented a general discussion of the reciprocal lattice in structure theory, and showed how atomic structure arrangements could be described by assigning weights, identical with the structure factors, to the points of the reciprocal lattice. This Fourier transform development was brought to its completion by Bienenstock & Ewald (*Acta Cryst.*, 1962, 15, 1253-1261) in a paper on the symmetry of Fourier space, in which the 230 symmetry groups of crystal space were expressed in terms of complex weights at the reciprocal lattice points. Ewald's delight in Fourier transforms also appeared in his discussion (*Proc. Phys. Soc.*, 1940, 52, 167-173) of the shape transforms of finite crystals, a topic considered also by Laue and Patterson.

Ewald's construction of the sphere of reflection and its intersections with the reciprocal lattice has proved immensely fruitful in the understanding of diffraction geometry and in the development of experimental methods, especially for rotation/oscillation and precession photography, and for diffractometers. An example of its current relevance will be described (Cruickshank,

Helliwell & Moffat, *Acta Cryst.*, 1987, A43, in press). The intense polychromatic radiation beams at synchrotron X-ray sources have brought renewed interest in the original Laue stationary-crystal method. Beautiful Laue diffraction photographs with many thousands of spots may be obtained with sub-second exposures, and present the possibility of following the course of kinetic experiments. Each spot may correspond to the exact overlap of many orders of a Bragg reflection (a matter discussed by Ewald). If the majority of spots are of multiple order, the Laue method would be of limited value in protein work. A theory of the distribution of multiple orders as a function of  $d^*_{\max}$ ,  $\lambda_{\max}$  and  $\lambda_{\min}$  has been developed, and it is found that typically more than 90% of the spots correspond to single orders.

Supplementary references

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11.X-5 CURRENT STATUS OF PHASE DETERMINATION BY MEANS OF MULTIPLE BRAGG SCATTERING. By Q. Shen and R. Colella, Department of Physics, Purdue University, W. Lafayette, IN. 47907, U.S.A.

The feasibility of multi-beam diffraction for determining phases of structure factors is assessed on the basis of recent experimental results. It is shown that the method works well in situations in which the global interaction between x-ray photons and crystal is weak, in which case diffraction takes place by single scattering events, and crystal perfection does not play a role in interpreting the experimental results. Three successful examples of phase determinations using the notion of Virtual Bragg Scattering are presented. One case is of particular interest, because the crystal ( $V_3Si$ ) is mosaic, and the phases were a priori unknown. Some problems and limitations of the method are encountered with molecular crystals, because their reciprocal space is densely populated, and their nodes (Bragg reflections) have very small sizes on account of the small values of the structure factors involved. We report here on a recent experiment performed at NSLS (Brookhaven National Laboratory) that successfully revealed the phase related asymmetry effect on the (202) reflection of an organic crystal (benzil:  $C_{14}H_{10}O_2$ ), by utilizing 3.5 keV soft x-ray radiation. A multi-beam calculation with mosaic spread included shows good agreement with the experimental data. Further analysis indicates that it is possible to extract arbitrary values of the phase angle from an experiment, for a noncentrosymmetric crystal, by using an analytical formula derived from a perturbation theory of the asymmetry effects.