11.X.1 CHARACTERIZATION OF DEFECTS IN X-RAY TOPOGRAPHY USING SIMULATION METHODS.

By J.Gronkowski, Institute of Experimental Physics, University of Warsaw, Poland.

The range of materials which can be studied by X-ray diffraction topography has increased significantly within the past few years due to progress in the quality of single crystals. On the other hand, the rapid development of computer hardware and software has reduced to a reasonable value the computing time needed to make a simulation of a topograph (Epelboin and Soyer, Acta Cryst., 1985, A41, 67-72). Thus, it would be possible now to intensify the use of the simulation techniques for the defect characterization. In the present paper possible new application fields of these techniques will be reviewed. Limitations of the method (partly inherent in the X-ray topography itself) will also be discussed (see Epelboin, Mat. Sci. Eng., 1985, 73, 1-43 for an excellent review). The advantages and drawbacks of making simulations in various topographic setups (plane wave and spherical wave, transmission and reflection case, stationary and traverse) will be compared. The future developments of the simulation techniques, especially in conjunction with the progress in synchrotron research will also be highlighted.

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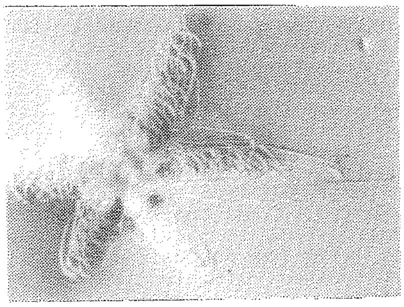

Fig. 1

Dislocation Loops around an Indent on a B type {111} Surface

11.X-2 CHARACTERISATION BY X-RAY TOPOGRAPHY OF PLASTIC DEFORMATION AROUND INDENTS ON INDIUM ANTIMONIDE

by M.R. Surowiec* and B.K. Tanner, Department of Physics, Durham University, South Road, Durham. DH1 3LE. England.

The dislocation configurations around microindentations on {111} and {001} surfaces of InSb have been studied by X-ray transmission topography. Both Lang topography and white beam synchrotron radiation topography were used. Marked differences are found between the configurations from indents on (001) and (00$\bar{1}$). Three types of loop were identified; (a) elongated loops on inclined {111} planes, with $\frac{1}{2}\langle 110\rangle$ Burgers vector and of screw-B(g) and screw-A(g) character in the long and short wings respectively, (b) near surface 60° prismatic dislocation loops, probably resulting from interactions of the former type, and (c) loops inclined to the specimen surface resulting from interactions between inclined loops on two {111} planes. The asymmetry in the configurations is explained by the different velocities of A(g) and B(g) dislocations; M. Surowiec and B.K. Tanner, Phil Mag. (1987) in press.

Configurations on (111) and ($\bar{1}\bar{1}\bar{1}$) also differ markedly. Glide occurs only on B type {111} planes. Extended loops occur around A surface indents, glide taking place on inclined {111} planes with an extended screw segment parallel to the specimen surface. Around B surface indents, glide occurs predominantly in the plane parallel to the surface (Fig. 1). Direct evidence for the formation of Lomer - Cottrell locks is found and the presence of many quarter loop segments provide evidence to support Alexander's (1979) model of dislocation association.

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11.X-3 INTRODUCTION: THE SIGNIFICANCE OF THE EWALD'S DYNAMICAL THEORY OF DIFFRACTION.

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Professor Paul P. Ewald was not only a great scientist but also a great teacher and organizer in our scientific community. Although this microsymposium is to be devoted to his scientific achievements, one can not withstand citing his Editorial Preface to Acta Cryst. (1948, 1, 1-2), which is indeed a historical document of IUCr. It shows clearly his foresightedness to crystallography and other sciences.

His greatness, however, is the synonym of our difficulty in organizing this symposium. What can be presented here would be merely an aspect of "elephant" figured out by a blind. It is hoped, therefore, for participants to build up the true image through other addresses and mutual conversations during the Congress.

The Ewald's theory: He started his scientific carrier in 1910 under A. Sommerfeld. His reminiscence is recorded in his article "The Origin of the Dynamical Theory of X-ray Diffraction (J. Phys. Soc. Jpn., 1962 Suppl. B-II, 17, 48-52)". He wrote up his dissertation by 1912, the year when M. von Laue et al. published the Nobel Prize work. Soonafter, his life work "Zur Begründung der Kristalloptik" appeared in following articles. The cores, however, can be found in the dissertation.

Teil I: Theorie der Dispersion. Ann. Physik. 1916, 49, 1-38. Teil II: Theorie der Reflexion und Brechnung, ibid. 1916, 49, 117-143. Teil III: Röntgenstrahlen, ibid. 1917, 54, 519-

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 aethetic 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.

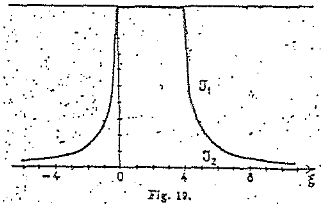

Fig. 19.

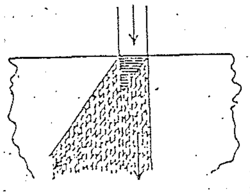

Fig. 21.

From Teil III cited above.

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}, λ_{max} and λ_{min} has been developed, and it is found that typically more than 90% of the spots correspond to single orders.

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Ewald, 1936, Z. Krist., 93, 396-398.

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,

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.