

14-Diffraction Physics and Optics

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The aim of this paper is to calculate the integrated reflectivity of a skew-symmetric triple-Laué interferometer under variable geometry conditions and with absorption. In these calculations we follow the path of Bonse & Graeff (1977) expanded by subunit rotations. Further we discuss the design of the interferometer used for the experiment, in which a new developed optical autocollimator (ACT) capable of resolving 0.000 01 sec of arc is calibrated by angular X-ray interferometry.

PS-14.03.05 MODIFIED BRAGG LAW FOR HETEROLAYER STRUCTURES. By W.A. Keller* and D.S. de Vasconcelos, Instituto de Física, Universidade Federal da Bahia, Salvador-Ba, Brazil.

X-ray diffraction patterns for stratified structures including epilayers and superlattice structure are analyzed by an approach which was first developed for the self-consistent EM scattering by a single plane of dipoles, considered as a unit of scattering. The rigorous vectorial waves solution for the σ - and π -states of polarization has previously been found for the scattering unit and extended to a whole crystal, represented by a stack of such units. The guiding principle was the simple demand, of continuity of EM field vectors between all the units. As a result, a modified Bragg law for a perfect big crystal was obtained. We now join the known solutions for homogeneous crystal structures to resolve the scattering problem for stratified structures, for which individual components can have origin in different crystal structures as, for instance, Ge and GaAs. Again, we use the same guiding principle of continuity of EM field vectors between all the components. By this approach it is possible to obtain diffraction profiles for selected structures, that previously could only be handled by some hybrid kinematic-dynamic types of approach (S. Bensoussan, C. Malgrange and M. Sauvage-Simkin, 1987, *J. Appl. Cryst.* **20**, 222 and A. Authier, J. Gronkowski and C. Malgrange, 1987, *Acta Cryst.* **A45**, 432).

The infinite multi-superlattice structures show the diffraction profiles with features such as a sequence of tophat curves for each satellite reflection (Fig.1a). The respective total reflection regions (TRR) depend, in a critical way, on the charge densities of the component units, their structure factors and the polarization state of the incident radiation. This dependence is of the same type as that observed for the main peak and it is preserved even in cases when TRR is reduced to fractions of the arc second. The angular region of the latter depends, for a given order of reflection, on chemical composition, homogeneous layer thickness, charge density value and inter- and intra-layer distances between scattering units. The finite multi-superlattice and multi-epilayer structures display diffraction patterns of the kinematic type. A continuous transformation of the diffraction-profiles from kinematic to dynamic type can occur as a result of a simple change of numerical value of two parameters, which depend on structure components, such as the layer thickness and the charge density of the respective component (Fig.1b).

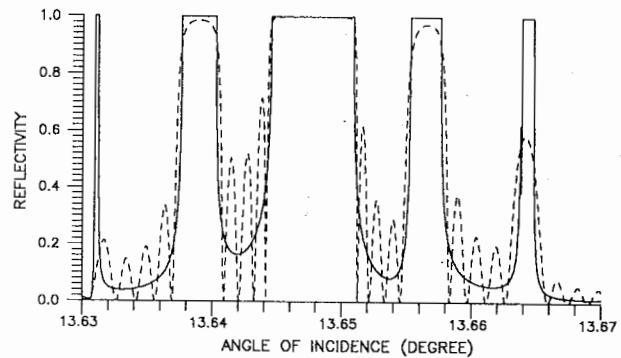


FIG.1: SUPERLATTICE STRUCTURE OF $1024*(111)\text{Ge}-700*(111)\text{GaAs}$
 — 1a INFINITE NUMBER OF UNITS
 --- 1b 4 UNITS

An attempt is made to formulate a modified Bragg law version for satellites for the multilayer superstructures with appropriate indices of refraction intrinsically included into the scattering model.

PS-14.03.06 AN EXACT AND ANALYTIC GEOMETRY OF BRAGG DIFFRACTION By Hsueh-Hsing Hung, Synchrotron Radiation Research Center, Taiwan

A novel interpretation of Bragg diffraction is reported. We have found a simple way to precisely reformulate the dynamical theory of diffraction so as to derive several important results with their clear geometric meaning on the well-constructed dispersion surface. Poynting vector is proved normal to the dispersion surface, on which a corrected hyperbola is proposed. By contrast with the conventional theories, our results not only propose a picture for the first time to cover the refraction (Fresnel's reflectivity) and diffraction (Darwin's curve) in all the angular range, but can be easily applied to the generic diffraction phenomena in periodic structure. The physics of Bragg diffraction is common in nature, the geometry should be expected simple. It is indeed and will be presented in this talk.

PS-14.03.07 DIRECT OBSERVATION OF DIFFRACTED X-RAY BEAM IN THE FORWARD DIRECTION FROM THIN AND IMPERFECT NATURAL DIAMOND CRYSTALS. By Krishan Lal*, S. Niranjana N. Goswami and Ajit Ram Verma, National Physical Laboratory, New Delhi - 110 012, India.

We have succeeded in direct observation and study of diffracted beams in the forward direction, in the case of thin

diamond crystals whose diffraction curve half widths were two orders of magnitude larger than the theoretical values for ideal structure. Specimen diamond crystals were (111) platelets of Type II variety with thicknesses varying in the range : 1.24 mm - 1.63 mm corresponding to μt values : 0.28 - 0.37. These were borrowed from the famous collection of Late Prof. C.V. Raman. A five crystal X-ray diffractometer developed in our group has been employed in a three crystal configuration with (+,-,+) geometry. A highly monochromated and collimated $\text{MoK}\alpha_1$ beam with very small width in the plane of diffraction was the exploring beam. A new technique for masking of residual direct beam and isolating bulk of the forward diffracted beam has been employed (LAL, GOSWAMI & VERMA, 1992, Solid State Commun. 81, 461-465). This technique enables us to separate the forward diffracted beam from the residual direct beam. The specimen crystals were quite imperfect with diffraction curve half widths for $(\bar{2}20)$ diffracting planes in the range: 100 arc sec - 280 arc sec. The photographs of the beams in the forward direction clearly show forward diffracted beam well resolved from the residual direct beam (Fig. 1). For the sake of comparison a topograph for this reflection is also shown in Fig. 1. By masking the residual direct beam, diffraction curves could be recorded with the forward diffracted beam. Fig. 2 shows a typical set of diffraction curves. Well defined peaks are observed.

The intensity of the forward diffracted beam decreases with the fall in the level of perfection. However, it could be observed even when diffraction curve half widths were ~ 280 arc sec.

We have also measured total transmitted intensity around the Bragg angle θ_B as a function of the glancing angle. It showed a notable increase at θ_B establishing a dependence of absorption coefficient μ on θ near θ_B and a substantial decrease of μ at θ_B .

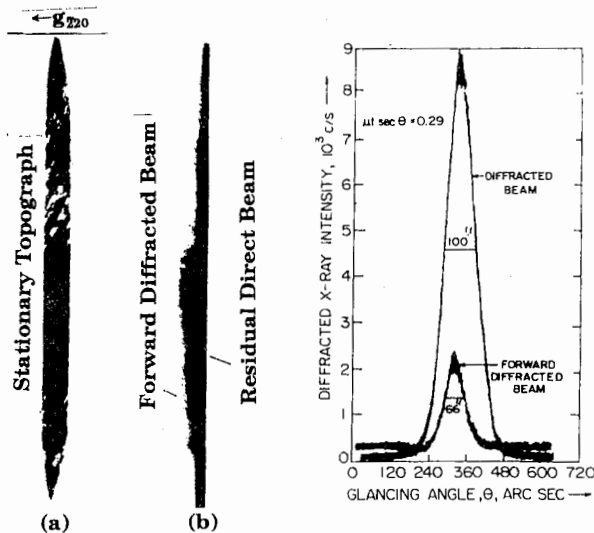


Fig. 1

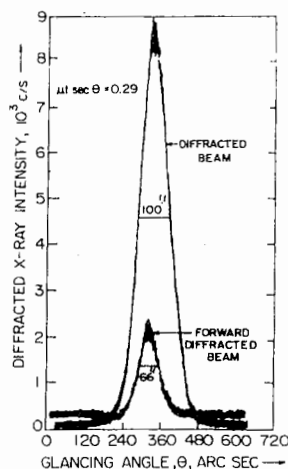


Fig. 2

PS-14.03.08 A NEW ANALYTICAL CALCULATION OF THE ABSORPTION DURING SCATTERING. By Roger C Clark and John S Reid,* University of Aberdeen, Departments of Mathematics and Engineering, Aberdeen AB9 2UE. Scotland.

A new mathematical method of evaluating the absorption during scattering is developed by applying Gauss's theorem and Stokes' theorem to the absorption integral. The resulting expression avoids the standard division of a polyhedral crystal into elementary tetrahedra, [MEULENAER, J. DE & TOMPA, H. (1965) Acta Cryst. 19, 1014 - 1018]. The method also points the way to a numerically robust algorithm for accurately evaluating the absorption and the mean path length. The results of implementing this method are illustrated. Not only can the absorption by normal convex polyhedral samples be evaluated but also inclined cylinders and spheres, in polyhedral approximation. The method is particularly efficient for energy-dispersive scattering, where the absorption is required for the same geometrical configuration at many wavelengths.

14.04 - X-ray Magnetic Scattering, Dynamical Diffraction

PS-14.04.01 DESCRIPTION OF MÖSSBAUER DIFFRACTION PATTERNS USING MULTIPOLE POLARIZABILITY TENSORS. By E.N. Ovchinnikova, Department of Physics, Moscow State University.

Mössbauerography is a diffraction method, whose great possibilities were proclaimed, but not realized yet. Individual experiments using this method have shown that, when the technical difficulties are overcome, Mössbauerography gives more valuable information than any other method. Apart from the technical difficulties, there is a problem of interpretation of the Mössbauer diffraction pattern. Its symmetry depends on the crystal structure, the hyperfine field structure and on the type of Mössbauer nucleus transition (E.N. Ovchinnikova, R.N. Kuz'min, *Comp. Math. Appl.*, 1988, 16, 657-661). Such complex symmetry leads to the appearance of purely magnetic, quadrupole and combined reflections in the Mössbauer diffraction pattern. In the present paper, we consider an adequate theoretical technique which allows to describe Mössbauer diffraction pattern features in a similar way as the Structure Factor $F(H)$ describes X-ray diffraction. It is shown that the multipole polarizability tensors $\hat{G}^L(H)$ must be used for this purpose. Their rank is equal to two for dipole nuclear transition and is greater for higher multipole transitions. Tensor representations of higher ranks are useful for considering the symmetry of $\hat{G}^L(H)$ tensors. They are constructed using the irreducible representations of a crystal space group. We also consider methods of construction of the multipole polarizability tensors in the cases of quadrupole, magnetic and combined hyperfine field structures in crystals.

PS-14.04.02

INDEX OF REFRACTION AS A DYNAMICAL VARIABLE IN THE SELF-CONSISTENT EM SCATTERING. By D.S. de Vasconcelos* and W.A. Keller, Instituto de Física, Universidade Federal da Bahia, Salvador-Ba, Brazil.

The self-consistent treatment, developed initially for X-ray diffraction in perfect crystals, is used to define the index of refraction