14-Diffraction Physics and Optics

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 & TIOMPA, 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 MULTIPLE 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. Mat. 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 G(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 G(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. do Vasconcelos* and W.A. Kodner, Instituto de Fisica, 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.

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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 α-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 MoKα 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 (220) 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 B and a substantial decrease of μ at θ B.

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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.