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 MoKα_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.

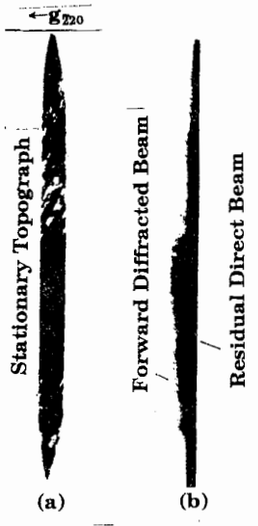

Fig. 1

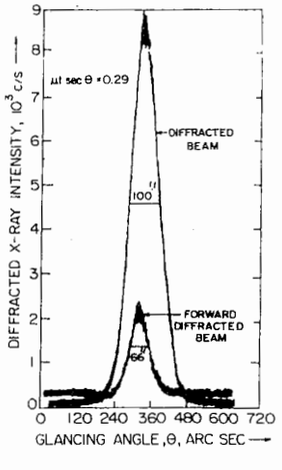

Fig. 2

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 polarizabilities 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

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as a dynamic parameter even in a region where the Bragg law is not valid. This index of refraction is a straight-forward consequence of using the self-consistent mode of interaction developed between light, represented by EM field, and matter, by a set of vibrating dipoles. In this mode of scattering the EM field forces dipole oscillations, whose field must be accounted for as well as external field, composed of two waves, the incident and the reflected. The dipole contribution allows the energy of the system (considered without absorption) to be conserved.

Refraction and absorption are treated separately and appear as 'macroscopic' type phenomena in directions parallel to scattering planes of dipoles and as 'microscopic' phenomena in the direction normal to them. The last property is a direct result of the approach developed herein which treats the plane of dipoles as an EM plane wave transformer, altering in a steplike manner the amplitude and the phase of both interacting waves. The change in phase mentioned causes the direction of energy flow to be different from the direction of the actual wave vector which gives rise to the appropriate index of refraction, which in turn is different from the direction of either of the interacting waves. The second reflected wave, though it appears as a macroscopic entity only in some special cases, always has an important role in microscopic EM fields (evaluated at the dipole level).

The calculated values of index of refraction for Si single crystals within this model are smaller than unity for X-rays and larger than unity for light of longer wavelength. This result appears for both states of polarization and does not depend on absorption. In the intermediary region, for given charge density and radiation wavelength, some critical point can always be found for which the index of refraction is exactly equal to unity.

PS-14.04.03 DYNAMICAL CALCULATIONS OF DIFFRACTION CONTRAST FROM MULTILAYER STRUCTURES AND CRYSTALS CONTAINING DEFECTS. By Y.J. Li*, S.Q. Wang and L.-M. Peng §, Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O.Box 2724, Beijing 100080, China. also §Department of Materials, Oxford University, Oxford OX1 3PH, U.K.

Recent years have seen the extension of the conventional two-beam diffraction contrast technique to many-beam cases. In particular the combination of the technique of convergent beam electron diffraction (CBED) and real space imaging of multilayer materials and crystals containing defects has put a demand for an efficient and consistent framework for analyzing the experimental results obtained under many beam diffraction geometry. In this paper we will present a many-beam matrix formulation of dynamical theory of electron diffraction by multilayer materials and imperfect crystals, and its applications to the many interesting systems, such as the Si/GeSi strained layer superlattice and crystals containing stacking fault and dislocations. The theoretical results obtained have been compared with experimental observations, and excellent agreement has been achieved. Comparing with the existing algorithms, our matrix method is more flexible for different diffraction geometries and strain field distributions, and is at least an order of magnitude more efficient. Dynamical high-order Laue zone (HOLZ) effects are also most conveniently included.

PS-14.04.04 THE EFFECT OF HIGHFREQUENCE ULTRASOUND ON THE DIFFRACTION OF THERMAL NEUTRONS IN BENT SILICON SINGLE CRYSTAL.BRAGG CASE. By E.M.Iolin, E.A.Raitman, V.N.Gavrilov, B.V.Kuvaldin*, Institute of Physics,Latvian Academy of Science, 229021, Latvia. Yu.A.Alexandrov, E.M.Galinsky, A.A.Loshkarev*, Joint Institute for Nuclear Research, 141980 Dubna, Russia. L.N.Sedlakova*, INF, Rzez, Chehia.

The influence of high-frequence ultrasounds on the reflection of neutrons with different wave lengths from bent silicon single crystals has been investigated.The frequency of ultrasound 30-150 MHz; neutron wave lengths 0,96A, 1,31A and 1,92A; radius of bending $R=5x10\text{-}5x10^4$ m.
The experiments were conducted by DIFRAN set up using time-of-flight methods.
The silicon sample with dimensions 6x60x120 mm^3 was bent by special arrangement. Simultaneously the intensity I_s of two reflections 220 and 440 was measured.
Under certain $R \approx 10^4$ m, the growth of I_s with amplitude of ultrasound wave increasing was changed drastically to the decrease which reaches up to 50% from the primary I_s. The set of minima connected with phonons-neutron interaction was observed.
The results were explained by dynamic scattering theory developed recently for Laue case (E.M.Iolin, E.A.Raitman et al. Sov. Phys. JETP, 1988, 67, 989). It has been shown that high-frequency ultrasound violates the adiabatic motion of excited points on the sheetsRof the dispersio n surface in slightly deformed single crystals. The good quantative agreement between theory and experiment was obtained. The possibilities of using of this effect will be discussed.