11.7-04 X-RAY DYNAMICAL THEORY OF DIFFRACTION AT BRAGG ANGLES NEAR $\pi/2$.*

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Some approximations normally used in the dynamical theory cease to be valid when the Bragg angle $\theta \simeq \pi/2$. Previous work by Kohra & Matsushita (Z. Naturf. (1972), 27a, 484) and recently by Brümmer, Hoche & Nieber (Phys. St. Sol. (a)(1979),53,565) dealt only with some partial aspects in the non-absorbing case. To solve this problem one writes the reflectivity as $R_P = R_P(y)$ with $y= y(\theta_c)$ and notices that $R_P(y)$ is independent of θ_b if y is conveniently chosen. After analysing the approximations adequate for $\theta \simeq \pi/2$ we obtained expressions for the various quantities of physical interest (k_o, k_h, R_P, etc.) whose analysis led to the distinction of three different regimes of diffraction. Case I: a limiting situation of the usual Bragg dynamical diffraction; Case II: a very peculiar transition regime and Case III: a case which tends asymptotically to the soft X-ray propagation. $R_P = R_P(y)$ was then calculated for a semi-infinite crystal and the transformation $y = y(\theta_o)$ established for this case: it turned out to be cubic in θ_o instead of linear as in the common case, having a local maximum in the region of high reflectivity. The profiles $R_P= R(\theta_o)$ are then doubled having another part which is nearly the mirror image of the first. It is shown that the linewidth W is of the order $\chi^{1/2}$, i.e., two or three orders larger than in the normal case where it is of order χ. When $\theta_b \equiv \pi/2$, $W = 2|\chi_h|^{1/2}$ in agreement with Kohra and Matsushita (op.cit.). The theory was applied to the diffraction of CoKα_1 by the 620 planes of Ge tuning the lattice parameters by means of the temperature in the range 8.7 to 13,0°C so as to reproduce the cases cited above. The following are results of general validity: (a) The large linewidths (several minutes of arc, order $\chi^{1/2}$) and large integrated intensities, reflectivities typically over 90%. (b) Very small effects of the orientation of the crystal surface (shifts of seconds of arc). (c) The decrease of linewidths as the temperature increases, the situation approaching that of the usual theory. (d) The asymmetry of peaks in case I. (e) A central depletion in case II. (f) A peculiar "square" shape obtained just when the central dip is eliminated. (g) The rapid decrease in reflectivity in case III. (h) The high sensibility of the profiles to small changes in lattice parameters implying its use for this purpose and that the actual experimental profile may depend upon the defects of the sample. (i) Attention is called to the possibility of having rather high intensities diffracted under "complex Bragg angles" (the case when the spheres of radius K centered at H and O do not intercept each other). (j) For a certain value of y, $\delta\theta_o = \delta\theta_b$, the beams returns exactly on the same line. The formalism introduced provides the basis for the design of X-ray resonant cavities.

Supported by FAPESP and CNPq (Grant nº 2222.1785/78).

11.7-05 OBSERVATION OF MULTI-BEAM BORRMANN EFFECTS ON THE DIRECT BEAM FROM SILICON FOR MoKα USING LANG CAMERA.*

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The forward diffracted (FD) and transmitted reflected (TR) images of simultaneous Borrmann diffraction from germanium single crystals for CuKα radiation are usually detected photographically by using the high resolution divergent-beam method. It is, however, difficult to apply this method to obtain intensity distribution of the FD beam for silicon, using CuK or MoK radiation, because of the high background of the direct beam due to white radiation and fluorescence. We report here that by using the Lang topographic camera with an appropriate slit system we are able to observe clearly on the direct beam the dynamical interaction effect of multi-beam Borrmann diffraction in silicon single crystals. The case of study is the 4-beam, (000)(400)(220)($2\bar{2}0$), for MoKα. The observed intensity enhancement on the FD beam at the exact 4-beam point agrees qualitatively with the calculation based on the plane-wave dynamical theory of X-ray diffraction. Detailed calculations about the diffracted intensities, dispersion surface, absorption, and the excitation of mode are also given. Due to the fact that the experiment needs a much shorter exposure time to X-ray than the divergent beam technique and that the present method is not strictly restricted to a certain material or radiation, it may be an advantage to adapt this method for solving the X-ray phase problem in the way proposed by Post [Post, B. Phys. Rev. Lett. (1977) 39, 760].

*Financial support from FAPESP is gratefully acknowledged.

11.7-06 A VARYING STEP ALGORITHM FOR THE NUMERICAL INTEGRATION OF TAKAGI-TAUPIN EQUATIONS.

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Various methods have been suggested for numerical integration of Takagi-Taupin equations (Taupin, (1964) Bull. Soc. fr. Minéral. Cristallogr. 87, 469-511 - Authier, Malgrange and Tournarie (1968) Acta Cryst. A24, 126-136). More recently Petrashen ((1976), Fiz. Tverd. Tela (Leningrad) 18, 3729-3731) has suggested a varying step algorithm to take into account the fast oscillations of the amplitude of the wave fields near the edges of the Borrmann fan. The main difficulty is in finding a method of adapting the local integration step to its best value.

We have developed a new algorithm based on the following considerations:

1.-Choosing of integration step is dependent upon the local value of the extinction distance. 2.-The interaction of a defect with the wave fields is weaker near the reflected edge of the Borrmann fan. 3.-The amplitude of the wave fields increases tremendously in the direction of the direct image of a defect whenever it exists.

We will study the condition of convergence of such an algorithm and compare it to the classical constant step algorithm. We will show that it enables us to take into account the direct image and that it is possible to simulate section topographs of very high accuracy. Moreover the computing time may be decreased by a factor from 3 to 10 as will be shown in some examples of dislocation images in quartz and silicon.

Simulation of section topographs using this new algorithm are faster and cheaper, which should allow the use of simulations in all laboratories.

Moreover, it will be necessary to use it for the simulation of translation topographs.