

11.7-1 ANIMATED SIMULATION OF THE PATHS OF THE WAVE FIELDS IN A CRYSTAL CONTAINING A DISLOCATION. by Y. Epelboin, C. Guidi-Morosini, F. Morris, A. Rimsky and A. Sover, Laboratoire de Minéralogie-Cristallographie, U.A.09 CNRS, Universités P.M. Curie et Paris 7, 75252 Paris Cedex 05, France

Simulation allows to simulate the contrast of a defect in X-Ray topography. It may also be used to understand the interaction between the wavefields and the deformed crystal in a plane of incidence (Y. Epelboin, Acta Cryst. A, 1979 35, 38-44) by computing the repartition of intensity in the Borrmann fan.

Since the computation is based on the integration of the Takagi-Taupin equations, it takes into account both curved wave fields corresponding to the Eikonal theory or geometrical optics and the diffraction or newly created wavefields.

We have simulated the situation for various positions of the core of a dislocation, where it crosses the incidence plane. The images have been drawn on a color picture system, using false colors to show the different levels of intensity. They are presented in a sequence which gives the impression of a movement, as if the dislocation was moving in the crystal. This animation, in conjunction with the use of colors, allows to follow the changes in the interaction between the wave fields and the defects when its position changes in the crystal.

It shows that the interaction is much stronger when the dislocation lies near to the refracted direction and that the position of the extinction fringes is already disturbed when the dislocation crosses the incidence plane far outside the Borrmann fan, but on the side of the refracted direction. The interaction decreases very rapidly when the dislocation moves outside the Borrmann fan, on the side of the reflected direction. When the defect crosses the refracted direction, the formation of the direct image is clearly visible.

When the dislocation lies inside the Borrmann fan, we found that the position of the extinction fringes is only modified at depths greater than the position of the core of the defect. This may be explained using the notion of wave packet (F. Balibar and C. Malgrange, Acta Cryst. A, 1975, 31, 425-434): it is necessary that the wave fields travel on a distance of the order of their modulation, i.e. the extinction distance Λ , to interfere with the distorted crystal.

The formation of the intermediary image of a defect is also clearly shown: the interaction is much stronger when the dislocation crosses areas where the extinction fringes present a maximum of intensity; thus, when the depth of a defect changes the intensity of the diffracted beam oscillates, giving rise to a set of fringes whose period is roughly the same than the extinction fringes.

This short movie summarises various situations where a defect interacts with the diffracted beam in a nearly perfect crystal. The animation is a very powerful means to understand the influence of a given parameter. In the present case we have shown the influence of the position of a dislocation in the formation of its contrast.

11.7-2 X-RAY STATIONARY WAVES IN THIN CRYSTALS. By A. Authier, Laboratoire Minéralogie Cristallographie, associé au CNRS et aux Universités PARIS VI et VII, 4 Place Jussieu, Paris - France.

The X-ray stationary waves technique for the localization of atoms at surfaces and interfaces is now quite widespread and has been used up to now with thick perfect crystals. As is well known, in this case, total reflection occurs at the Bragg incidence on non absorbing crystals and one wave field only is excited at a time. As the crystal is rocked, this excited wave belongs first to one branch of the dispersion surface and then to the other one. The 180° phase difference between these two branches accounts for the correlated shift of the nodes and antinodes of the stationary waves which is used to explore the unit cell. It is interesting to find out whether the same method can be used in the case of thin crystals and whether geometrical theory of diffraction is a good approximation for very thin crystals. It is also well known that in the Bragg case for thin crystals two points are always excited simultaneously on the same branch of the dispersion surface. The stationary waves are thus modulated by the Pendellösung oscillations. Traditional two beam dynamical theory for absorbing crystals was used to calculate the total intensity of the field at the crystal surface and within the crystal, taking Pendellösung into account and its variations with the position within the unit cell, the angle of incidence, the total crystal thickness and the depth within the crystal. The integrated fluorescent yield over the crystal thickness was also calculated. The results for a crystal thickness equal to one extinction distance are very similar to those for a thick crystal with only a small modulation. For a crystal thickness down to one tenth of an extinction distance, this modulation becomes very important. However, even then the signals from different positions within the unit cell are easily distinguished. For example, the signals from the arsenic and gallium positions from a 111 GaAs surface are quite different and complementary. This is true both for the signals from the crystal surface and for the integrated signal from the whole crystal thickness. Even for such thin crystals the influence of absorption is significant for highly absorbing crystals. The results obtained using geometrical theory of diffraction are quite different from those obtained using dynamical theory. This is not surprising since the variation of the phase of the reflected wave with the angle of incidence is given in the case of geometrical theory by that of the Fourier transform of the shape of the crystal while in the case of dynamical theory it is due to the interaction of the crystal structure with the electromagnetic wave. If the geometrical theory does give a good approximation of the reflected intensity for very thin crystals, it cannot therefore give information from which the phase can be directly obtained such as is the case for the position of nodes and antinodes of stationary waves. For this, dynamical theory is absolutely needed even for very thin crystals.