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.Soyer,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 Université 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.