Determination of the Burgers Vector of Perfect Dislocations Observed by X-ray Topography in Hexagonal Single Crystals

BY C. G'SELL
Laboratoire de Physique du Solide, L.A. au CNRS No. 155 ENSMIM, Parc de Saurupt 54042, Nancy, France

AND Y. EPELBOIN
Laboratoire de Minéralogie-Cristallographie, associé au CNRS Université P. et M. Curie, 75230 Paris CEDEX 05, France

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Abstract

Individual dislocations were observed in high-quality cadmium and zinc single crystals by means of transmission X-ray topography. The contrast of their images was characterized on the topographs as a function of the direction of the line, the Burgers vector and the diffraction vector. In addition, the theoretical contrast of perfect dislocations with all the possible Burgers vectors of the hexagonal lattice was computed by using a program which takes into account the crystal anisotropy. The comparison of experimental and theoretical results showed unambiguously that the long dislocation lines contained in the crystals have an a-type Burgers vector, while the loops and spiral dislocations have either a c- or c+a-type Burgers vector.

I. Introduction

Individual dislocations could be observed by transmission X-ray topography (i.e. Lang's method) in nearly perfect cadmium and zinc single crystals. These observations made possible the study of the dislocation movements (climb and glide) while the crystals were subjected to an oxidation (Fourdeux, Bergezhan & Webb, 1960; Michell & Ogilvie, 1966; Badrick & Puttick, 1971; G'Sell & Champier, 1975), a temperature variation (G'Sell & Champier, 1976) or a mechanical stress (G'Sell, 1977). All these authors showed that the dislocation images exhibit on the topographs a complex contrast which cannot be interpreted by the simple extinction criteria usually used in the case of cubic crystals. Strong residual contrast made difficult the identification of dislocations with Burgers vector \( e = [0001] \) and \( e + a = \frac{1}{2}(1123) \) when they were observed on a few topographs only.

Due to the high perfection of our crystals, it was possible to make a systematic study of the dislocation contrast on a large number of topographs obtained with different reflexions. In addition a computer program was used for the theoretical calculation of the direct image contrast in anisotropic crystals (Epelboin & Ribet, 1974). Correlation of both approaches made possible the determination of practical rules to identify the Burgers vector of all the dislocations of a crystal.

II. Observation of the dislocation contrast

The dislocation observed in the crystals can be classified into three types according to their contrast on X-ray topographs:

(i) The long linear dislocations, both grown-in and introduced by plastic deformation, exhibit narrow images whose contrast does not depend very much on the line direction in the basal plane (0001). Each dislocation disappears completely on one 1010 topograph. The six topographs in Fig. 1 show four linear grown-in dislocations in a cadmium single crystal. One of them emerges at both ends at the crystal surface. The three others react at a point where they form a triple node. The independent segment is totally invisible on the 0110 topograph. The three segments interacting at the node are invisible respectively on the 0110, 1010 and 1100 topographs. All the lines exhibit some contrast on the 2110, 1210 and 1120 topographs. It is to be noted that the contrast of a given dislocation is enhanced on the 2110 topograph whose diffraction vector is perpendicular to the diffraction vector of the 0110 topograph on which it is not visible.

(ii) The dislocation loops and spirals which are also contained in some crystals never completely disappear on the topographs. However, the contrast of these lines depends on their orientation in the loop or the spiral. For some of them, their contrast on the different 1120 or 1010 topographs may be deduced by a simple rotation of the image around the \([0001]\) axis. This property is illustrated by the six topographs in Fig. 2 which show the contrast of a hexagonal-shaped loop in a zinc single crystal. The portions of the loop parallel to the diffraction vector are invisible. The remaining parts of the loop show a strong residual contrast. Because of the hexagonal shape of the loop (whose sides are parallel to the \((1120)\) directions), only the corners are out of sight on the 1010 topographs, while
complete opposite sides disappear on the 1120 topographs.

(iii) A final type of contrast is exhibited by other loops and spirals whose image does not simply change from one topograph to another by a simple rotation. An example is given in Fig. 3 where a spiral is seen on six 1010 and 1120 topographs. On the 0110 topograph, the line disappears completely in the places where it is parallel to the diffraction vector. On the two other 1010 and 1100 topographs, the contrast only partially fades for the same condition. This aspect is also observed on the 1210 and 1120 topographs. Lastly, on the 2110 topograph the contrast is very strong all along the line.

III. Theoretical calculation of the dislocation contrast

Apart from some particular rhombus loops observed to appear in zinc crystals during an oxidation (G'Sell & Champion, 1975) the loops and spiral dislocations contained in our crystals never presented any internal contrast associated with a stacking fault. It can therefore be concluded that the configurations described above are perfect dislocations whose Burgers vector must be taken out of the three energetically favourable types of the hexagonal lattice:

\[ \mathbf{a} = \frac{1}{3}(1120), \]
\[ \mathbf{c} = (0001), \]
\[ \mathbf{c} + \mathbf{a} = \frac{1}{3}(1123). \]

All the topographs shown in Figs. 1, 2 and 3 were obtained with the K\(\alpha_1\) radiation from a Ag X-ray tube anode. Because of the thinness of the crystals \(t = 100 \mu\text{m} \approx 1/\mu\), the dislocation contrast is mainly due to their direct image (Authier, 1967).

In order to interpret the experimental results, the theoretical width of each dislocation's direct image was computed as a function of its Burgers vector and line direction. This computation uses a program which takes into account the diffraction conditions and the

Fig. 1. Contrast of dislocations of Burgers vector \(\mathbf{a}\) in a cadmium single crystal. (a) 0110, (b) 1010, (c) 1100, (d) 2110, (e) 1210, (f) 1120, (g) Burgers vectors of the three dislocations interacting at the node.

Fig. 2. Contrast of a prismatic hexagonal loop of Burgers vector \(\mathbf{c}\) in a zinc single crystal. (a) 0110, (b) 1010, (c) 1100, (d) 2110, (e) 1210, (f) 1120.
anisotropic elastic properties of the hexagonal metals (Epelboin & Ribet, 1974).

It is considered that the direct image of a dislocation is due to the extra reflexion, by an elastically strained region around the dislocation, of incident X-rays which do not fulfil exactly the Bragg condition for the perfect crystal. This active strained region is the region where the reflecting planes have a misorientation greater than the half-width of the reflection curve of the perfect crystal, that is

$$\delta(\Delta\theta) \geq \frac{2|C|}{\sin 2\theta} \left( \frac{2h}{\gamma_0} \right)^{1/2} \left( \chi_h \chi_k \right)^{1/2},$$

with $\theta =$ Bragg angle for the selected reflexion, $|C| =$ incident wave polarization,

$$\gamma_0 = \cos \left( z, S_0 \right),$$

$\chi_h = \cos \left( z, S_h \right),$ (see Fig. 4)

$\chi_h$ and $\chi_k =$ Fourier coefficients of the dielectric susceptibility of the perfect crystal.

The departure from Bragg incidence angle of the deformed planes is expressed by the relation (Authier, 1967)

$$\delta(\Delta\theta) = -\frac{\lambda}{\sin 2\theta} \frac{\partial}{\partial S_h} \left[ g . u(r) \right],$$

with $\lambda =$ wavelength of the X-rays,

$g =$ reciprocal diffraction vector,

$u(r) =$ displacement vector at a point defined by the vector $r$.

The strained region responsible for the creation of the direct image is then

$$\frac{\partial}{\partial S_h} \left[ g . u(r) \right] > \frac{2|C|}{\lambda} \left( \frac{2h}{\gamma_0} \right)^{1/2} \left( \chi_h \chi_k \right)^{1/2}.$$

For a section topograph (fixed crystal) the flat X-ray beam cuts this strained region along the area noted $S$ in Fig. 5. The reflected X-rays project this area onto the photographic plate (the plane of the topograph). The computer program was designed to draw on a line printer the enlarged shape of the projected area $P$. To complete the information about the active strained region, the computer draws also its sections parallel to the incidence plane $(Q)$ and perpendicular to the

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Fig. 3. Contrast of a spiral dislocation of Burgers vector $c + a$ in a cadmium crystal. (a) 01T0, (b) 1010, (c) 1100, (d) 21T0, (e) 1210, (f) 1120.

Fig. 4. Geometry of directions and angles in transmission X-ray topography.

Fig. 5. Principle of the direct image formation in transmission X-ray topography.
The kinematical theory applied in this paper is only an approximation, as shown experimentally by Miltat & Bowen (1975), but one may assume that it is good enough to obtain a close approximation to the dislocation contrast. It is assumed furthermore that the contrast of the real dislocation images is proportional to the computed image width.

IV. Comparison between experimental and theoretical results

The computation of the image width of dislocations was performed in the case of cadmium crystals with all the possible combinations of the following parameters:

- Burgers vectors:
  \[ a_1 = \frac{1}{3}[2110], \quad a_2 = \frac{2}{3}[2110], \]
  \[ c = [0001], \quad c + a_1, \quad c - a_1, \quad c + a_2, \quad c - a_2. \]

For a translation topograph (incident beam sweeping the crystal) the direct image of the whole dislocation line can be constructed from the area shape in the plane \( P \) of the topograph. As the incident beam sweeps the entrance surface of the crystal, successive sections \( S \) of the strained area produce successive images on the topograph. The theoretical width \( L \) of the direct image in a translation topograph can thus be obtained by translating along the projected direction of the dislocation line the area \( P \) drawn by the computer in the plane of the topograph (Fig. 7).

The computation is made in the case of linear anisotropic elasticity and the strain tensor around the dislocation is calculated by Stroh’s (1958) theory.
Dislocation line orientation: 18 directions in the basal plane for \( \alpha = 0 \) to 170° in order to explore all the orientations of the line of a dislocation loop.

- Diffracting planes: (2110) and (0110).

The 180 cases thus defined cover all the other ones by considering the symmetry of the hexagonal lattice.

Figs. 8 and 9 show the variations of the theoretical image width \( L \) with the previously defined parameters. In order to use these results more conveniently, the deduced contrast of a dislocation loop was drawn in Fig. 10 for the different combinations of Burgers vectors and reflecting planes.

By comparing this set of drawings with the topographs obtained experimentally, it can be seen that the agreement is quite good and that the three types of contrast described at the beginning of this paper can be associated respectively with the three Burgers vectors \( a, c \) and \( c + a \). It is also possible to identify the Burgers vectors \( a_1, a_2, \) and \( a_3 \), as well as the Burgers vectors \( c \pm a_1, c \pm a_2, \) and \( c \pm a_3 \). In the case of the long dislocations in Fig. 1 the \( a \) type of the Burgers vector could have been deduced without any computation from the simple extinction criterion \( g \cdot b = 0 \) which indicates also that the contrast of the three dislocations interacting at the node is consistent with three Burgers vectors whose sum is zero. However, this extinction criterion cannot be applied any longer in the case of the loops and spiral dislocations with Burgers vectors \( c \) and \( c + a \) because of their strong residual contrast. The criterion \( (g \cdot b \times t = 0) \) is often considered additionally but it gives only an approximate condition of non-visibility of the dislocations. It may suffice to elucidate the contrast of the \( c \)-type loops but cannot lead to reliable conclusions in complex situations such as the \( c + a \) spirals. The computation presented here is particularly useful in such cases. For example, one can find from the calculated image width curves of Fig. 10 that the contrast of the spiral in Fig. 3 is consistent with a Burgers vector \( c \pm a_1 \).

V. Determination of the sense of the Burgers vector

A more detailed analysis of the dislocation contrast can give additional information concerning the sense of the Burgers vector for a dislocation having an edge character. The topograph of Fig. 11 was obtained with a cadmium crystal using the \( K_\alpha \) radiation of a Mo X-ray anode (\( \mu \times t = 2.55 \)). It is seen that the contrast of the spiral is asymmetrical. The left side of the spiral (side of the diffraction vector \( g \)) shows a triple bright-dark-bright contrast while the right side shows an inverse dark-bright-dark contrast.

Applying the results of Hart & Lang (1963) and Lang & Polcarova (1965), based on the theory of Penning & Polder (1961), we suggest that the extra half planes of this prismatic dislocation could lie at the outside of the spiral curvature. By choosing a definite sense along the line, this information would fix the sense of the Burgers vector.

This analysis is also possible with the topographs obtained with the Ag \( K_\alpha \) radiation, though the contrast asymmetry, due to the dynamical images of the dislocation, is not so pronounced. These dynamical effects are responsible for the contrast asymmetry of the loop in Fig. 2 whose side pointed at by the \( g \) vector is less dark than the other side. This loop, of Burgers vector \( c \), is then also of a vacancy type, like the spiral shown previously.

A complete analysis, taking into account both curved wave fields and diffracted wave fields (Balibar, 1968) would need the simulation of the image of the dislocation by integration of Takagi's equation (Epelboin, 1974).

VI. Conclusion

The contrast of all the dislocations observed by X-ray topography in zinc and cadmium single crystals can be explained by considering mainly the kinematical
contrast of their direct images. It is thus possible to identify unambiguously the Burgers vector direction of the dislocations. The vacancy type of prismatic loops and spirals can be determined by additional dynamical effects.

The authors can supply interested readers with two versions of the computer program used in this work. One is a batch version and the other a conversational one.

References