

X-ray Topographic Determination of the Sense of Pure Screw Dislocations

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Early experiments^{1, 2} with crystals of calcite, silicon, and, in particular, germanium and silver chloride, taken under conditions such that the product of absorption coefficient (μ) and crystal thickness (t) was greater than 1, showed a *difference* in contrast between hkl and $\bar{h}\bar{k}\bar{l}$ topograph images of edge (or mainly edge) dislocations. Later experimental and theoretical studies^{3, 4} verified that this difference revealed the *sense* of the dislocation BURGERS vector. The ability to determine both the *sense* and *direction* of dislocation BURGERS vectors is useful in investigating the origin of dislocation configurations, as, for example, those in melt-grown crystals⁵. This contrast difference between hkl and $\bar{h}\bar{k}\bar{l}$ images of dislocations is well explained by the theories of PENNING and POLDER⁶ and KATO^{7, 8}. It arises from "wave point migration" on the dispersion surface (and consequent curvature of X-ray paths) in the long-range strain field of the dislocation, and occurs under conditions of appreciable anomalous trans-

mission⁹ so that waves belonging to branch I of the dispersion surface are dominant. The effect is noticeable in the outer parts of the dislocation image which correspond to crystal regions where the curvature is *not* sufficient to cause scattering of waves between branches I and II of the dispersion surface. Theory¹⁰ and experiment show that in the case of pure screw dislocations there is no difference between hkl and $\bar{h}\bar{k}\bar{l}$ images when no interbranch scattering occurs, i. e. in the outer parts of the dislocation image. (An exception arises if the dislocation approaches or intersects crystal surfaces in such a way as to destroy the symmetry of its long-range strain field: a difference between hkl and $\bar{h}\bar{k}\bar{l}$ images does then reveal its sense⁹.)

Now, under the conditions usually applying in the author's experiments, part of the strong "direct image" of dislocations is produced by interbranch scattering of radiation already undergoing BRAGG reflection by the perfect crystal matrix at angles close to the BRAGG angle. It may be predicted that in the case of pure screw dislocations this scattered radiation will introduce an asymmetry into the dislocation image profile, opposite in hkl and $\bar{h}\bar{k}\bar{l}$ reflections and dependent upon BURGERS vector sense, provided that appreciable anomalous transmission occurs and certain geometrical conditions are satisfied.

¹ A. R. LANG, Acta Cryst. 12, 249 [1959].

² A. R. LANG, J. Appl. Phys. 30, 1748 [1959].

³ M. HART, Ph. D. Thesis, University of Bristol 1963.

⁴ M. HART and A. R. LANG, Acta Cryst. 16, A 102 [1963].

⁵ A. R. LANG and M. POLCAROVÁ, Proc. Roy. Soc., Lond. A, in press.

⁶ P. PENNING and D. POLDER, Philips Res. Rep. 16, 419 [1961].

⁷ N. KATO, Acta Cryst. 16, 282 [1963].

⁸ N. KATO, J. Phys. Soc. Japan 18, 1785 [1963]; 19, 67, 971 [1964].

⁹ G. BORRMANN, Phys. Z. 42, 157 [1941]; Z. Phys. 127, 297 [1950].

¹⁰ N. KATO and Y. KAMIYA, to be published.

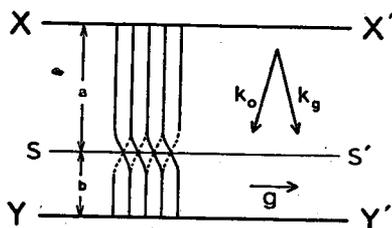


Fig. 1. Section of crystal in plane of incident wave vector k_0 and diffracted wave vector k_g . XX' is X-ray entrance surface, YY' is X-ray exit surface. Right-handed pure screw dislocation SS' is parallel to reciprocal lattice vector g . Distorted lattice planes above plane of diagram are shown schematically by solid lines, those below by interrupted lines.

Consider the symmetrical LAUE (transmission) geometry of Fig. 1 which shows the plane of incident and diffracted rays containing a pure screw dislocation SS' . Assume that the distances, a and b , respectively, of SS' from the entrance surface XX' and exit surface YY' are always large enough so that the influence of the surface on the dislocation strain field can be neglected. The BRAGG planes are drawn schematically: solid lines are above the plane of the diagram, nearer to the observer; interrupted lines are below. Thus SS' is a right-handed screw. Fig. 2 shows the region of the dispersion surfaces involved in the reflection g , drawn for one polarization mode only, for simplicity. Assume that a coherent spherical wave¹¹ is incident upon XX' .

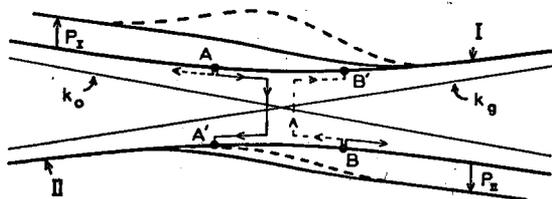


Fig. 2. Section of dispersion surface showing migration and jumping of wave point A to A' in distorted crystal above plane of Fig. 1, and of wave point B to B' in distorted crystal below plane of Fig. 1. Excitation of wave points in undistorted crystal schematically indicated by P_I above hyperbola I, and by P_{II} below hyperbola II. Continuous line, no absorption; interrupted line, appreciable anomalous transmission but normal absorption not included.

Then the excitation of wave points on the dispersion surface may be diagrammatically represented as shown. The excitation, P_I , of branch I is plotted as displacement above the branch I hyperbola as base-line, and the excitation, P_{II} , of branch II is plotted as displacement below the branch II hyperbola. Continuous lines represent the case of no anomalous transmission.

As the X-rays enter the strain field of the dislocation, all wave points, on both branches I and II, migrate at equal rates right or left along the hyperbolae. Consider the conjugate wave points A and B, both strongly and equally excited, and which correspond to rays travelling through the crystal near the k_0 direction. In the

strain field on the side of the dislocation above the plane of Fig. 1, A and B move to the right, as shown by continuous lines on Fig. 2. Closer to the dislocation the lattice curvature is strong enough to cause inter-branch scattering, or "jumping". The tie-lines connecting points on branches I and II between which jumping occurs are parallel to the strain gradient and thus appear vertical on the dispersion surface section shown in Fig. 2. The important jumping in the present case occurs near the apex of the hyperbola: a representative jump for the wave point originally at A is indicated. Energy is transferred from the more strongly to the more weakly excited branch: as drawn this would be from branch I to branch II. On leaving the strain field, all wave points move back to the left, so that the final result is that energy has been transferred from A to A'; and A' corresponds to a ray travelling through the crystal near the k_g direction. For the strain field below the plane of Fig. 1 the migration and jumping follows the interrupted line on Fig. 2 and is just the inverse of that described above. Thus the dislocation image is symmetrical about the dislocation line.

Now suppose $\mu a > 1$ so that anomalous transmission is appreciable. Neglecting the effect of normal absorption, the excitations P_I and P_{II} at a distance a from XX' will be roughly as shown by the interrupted curves in Fig. 2. A is now more strongly excited than B, and more energy is transferred from A to A' in the strain field above the plane of Fig. 1, than is transferred from

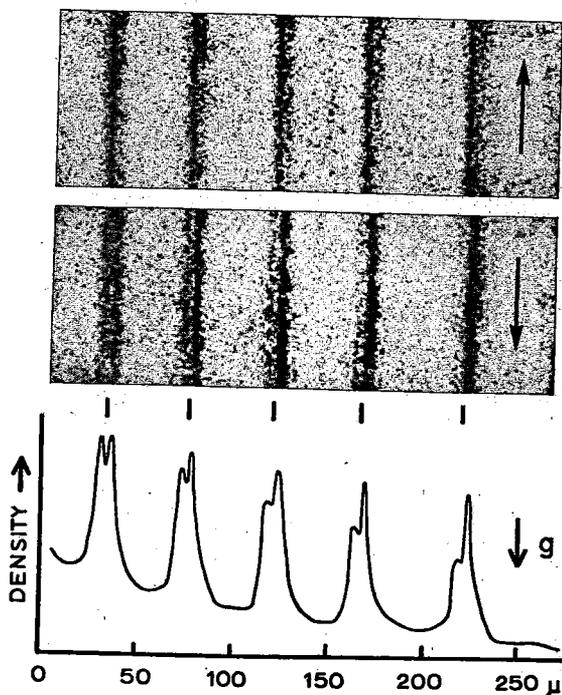


Fig. 3. Topographs of array of pure screw dislocations. $MoK\alpha_1$ radiation. Above, 220 reflection; below, 220 reflection and densitometer record of 220 topograph. Arrows indicate direction of reciprocal lattice vector. In this field μb is about 0.6 and is constant, on left $\mu a \approx 1$ and on right $\mu a \approx 1.6$.

¹¹ N. Kato, Acta Cryst. 14, 526, 627 [1961].

B to B' in the strain field below the plane of Fig. 1. If μb is quite small, this difference in excitation of A' and B' will be little changed at the exit surface. The dislocation image will be asymmetric, being stronger on the side above the plane of Fig. 1 than on the side below.

In practice, the images of pure screw dislocations normal to the BRAGG planes in f.c.c. structures, seen under the conditions $g \cdot b = 2n$, show double peaks. This helps to make asymmetry visible. Asymmetry just as expected has been observed in an array of pure screw dislocations forming one sector of a FRANK-READ "spiral" already described¹². Fig. 3 shows segments of five screw dislocations, in the 220 reflection, above, and in the $\bar{2}\bar{2}0$ reflection, below. In this field b is constant at about 0.4 μ m, and a increases from about 0.7 μ m in the top left to just over 1 μ m in the bottom right. The microdensitometer trace across the 220 field shows the

transition from the symmetrical case [$(a-b)$ small] to the asymmetrical case [$(a-b)$ large] quite clearly, despite some instrumental broadening in the trace. It follows that these screws are right-handed.

With these and other pure screw dislocations it is observed, in accord with prediction, that if a and b differ little, even if $(a+b)$ is large, no difference in the hkl and $\bar{h}\bar{k}\bar{l}$ images is apparent. With $b > a$ the asymmetry would be expected to reverse, for a given sense of BURGERS vector, but the images of dislocation with $b > 1 \mu$ m cannot be measured accurately. It has been observed that the apparent diameter of hexagonal loops, measured between the centres of gravity of the images of the screw segments, differs in the expected way on the 220 and $\bar{2}\bar{2}0$ topographs when a exceeds b sufficiently. This brief analysis neglects Pendellösung oscillations, but in the thickness range covered in Fig. 3 these oscillations are quite weak.

¹² A. AUTHIER and A. R. LANG, J. Appl. Phys. 35, 1956 [1964].

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