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DISLOCATION MOVEMENT IN DISTORTED CRYSTALS

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Résumé. — On démontre que la méthode topologique communément utilisée pour définir le vecteur de Burgers d'une dislocation, peut conduire à violer la loi de conservation du vecteur de Burgers dans les cristaux distordus. La solution proposée ici est de considérer la stabilité d'une dislocation comme une propriété physique du réseau qui impose le module du vecteur de Burgers et son orientation par rapport au réseau. Si d'autre part le vecteur de Burgers est conservatif dans l'espace euclidien, la loi de conservation géométrique est rigoureusement assurée. Avec ce modèle, il est nécessaire de considérer tout changement de l'orientation ou du module du vecteur de Burgers comme causé par l'éclatement de dislocations partielles qui peuvent être stables ou pas. Les vecteurs de Burgers des dislocation stables laissées, dans chaque cellule unité, sur un plan de glissement incliné, par une dislocation stable, peuvent s'exprimer au moyen d'un changement de métrique et du vecteur de Darboux le long des trajectoires décrites par chaque point de la ligne de dislocation sur le plan de glissement incliné.

Summary. — It is demonstrated that the topological method of defining the Burgers vector of a dislocation, which is at present commonly used, may lead to violation of the α Burgers vector conservation law » in distorted crystals. The remedy proposed here is to consider the stability of a dislocation as a physical property of the lattice which prescribes the Burgers vector modulus and orientation relative to the lattice. On the other hand, if the Burgers vector is considered as conservative relative to Euclidean space, the geometrical conservation law is rigorously ensured. It is necessary in this model to regard any change in Burgers vector orientation or modulus as being caused by splitting off partial dislocations that may be stable or not. The Burgers vectors of the unstable dislocation left in each unit cell on a bent glide plane by a stable dislocation may be expressed in terms of the changing metric and Darboux vector along the trajectories described by each point of the dislocation line on the bent glide plane.

Introduction. — It is generally accepted that if a crystal is bent, the dislocations in it that would have moved on straight slip planes in the undistorted crystal will continue to glide on the bent slip planes in the distorted crystal. Direct experimental evidence supports this view, as dislocation movement in heavily bent thin foils has in fact frequently been observed in the electron microscope, and, of course, in any bending experiment performed on single crystals or polycrystals the dislocations glide exclusively on the bent crystal planes. Accordingly, the method invented by F. C. Frank [1] of determining the Burgers vector of a dislocation by comparing the Burgers circuit described around the dislocation in the « bad » crystal that contains it with the same circuit, consisting of the same steps from lattice point to point in a « good » reference crystal is insensitive to rotation or dilatation of the « bad » crystal.

We might add that this is not surprising : the procedure for describing circuits on surfaces is a most familiar one in topology. Frank's method of comparing Burgers circuits is essentially topological, and it brings out well the topological oddity of the « bad » crystal containing the dislocation. It does not — and it cannot — predict that a dislocation will be stable, nor does it specify in what sense a « Burgers vector conservation law » would hold; it does only give a topological definition of a dislocation of which the quantitative properties still have to be established. To unambiguously achieve the latter is a difficult task, especially so for partial dislocations. It may be emphasized here that there is no topological difference between perfect and partial dislocations as is sometimes implied.

Surprisingly, it does not seem to be well-known that Burgers circuits can be described with equal precision around a partial dislocation as around a perfect one by applying a simple expedient. It consists in subdividing the interatomic distances in such a way that not only lattice sites actually occupied by atoms are given, but in addition those of the same lattice that might be occupied if stacking faults or twins would occur; in this manner a "common" lattice is defined. If, for instance, lattice points are described to the b. c. c. lattice along the <111> directions at 1/6 a <111> spacing, the partial dislocations bordering the twins and stacking faults commonly occuring in that lattice on $\{112\}$ planes could be described by Burgers circuits consisting of successive steps from common lattice point to common lattice point, whether occupied or not, in precisely the same fashion as perfect dislocations are described by Burgers circuits connecting occupied lattice points. Figure 1 illustrates the method ; it may some of the results of this approach as suspicious. There is, for instance, the curious limitation on the types of crystals that may be taken into consideration enunciated by Frank [2]: they should not be « Möbius crystals », by which the crystal configurations shown in figure 2 were meant. This exception was, introduced because otherwise it would be impossible « to have a single-valued correspondence between directions in the real crystal and in the reference lattice ». This requirement was taken over later by Bilby, Bullough



FIG. 1. — Projection of the b.c.c. lattice on $\{110\}$. By defining a «common» lattice of points that may be occupied by the normal lattice and by its twin, a normal Burgers circuit can be described around a twinning dislocation (Fig. a) or a partial dislocation (Fig. b) in the common lattice.

be verified that no closure on the stacking fault or twin boundary is required, as in the method at present commonly used. It may be concluded that topologically no difference exists between a partial and a perfect dislocation.

The failure of the law of Burgers vector conservation. - The term « conservation of Burgers vector » is often employed in various shades of meaning. It is the conservation law that is invoked both for explaining why an edge dislocation spontaneously cannot start to move on a new glide plane without having first taken part in a dislocation reaction, and for explaining why the same dislocation will move on a curved glide plane without undergoing any dislocation reaction. It is used to make clear that no single dislocation can be created spontaneously inside a crystal, and it is implicitly assumed in any dislocation reaction equation. Indeed, the whole concept of a Burgers vector would be devoid of meaning or value if it could not be regarded as a conservative physical vector quantity.

Nevertheless, the question may be asked whether the topological approach is complete and unexceptionable. In fact, there are reasons for regarding and Smith [3] in their article on « surface dislocations » This consideration is entirely correct, and from the point of view of the topological method it is a sensible and cautious requirement, as will be demonstrated in what follows, but on the other hand, one may well ask whether it is at all logically consistent to require that a crystal should :



- a) be « simply connected », and :
- b) contain dislocations.

The question is whether the fact that a crystal contains a dislocation does not automatically render it « multiply connected ». If the holes in the « Möbius » solids are « shrunk away » Somigliana dislocations

are left in the crystals. These dislocations exert the same long-distance influence as an array of ordinary Volterra dislocations, which may replace the Somigliana dislocations. No proof was given by either Frank or Bilby and coworkers (loc. cit.) that excepting the « Möbius » solid is permissible for a crystal that is supposed to contain dislocations.

It must be remarked, parenthetically, that the topology of crystals is not an established discipline comparable to the topology of surfaces. Although the term « Möbius » crystal is used with some confidence and although we are intuitively sure that such a crystal is very different from an « ordinary » torus made of the same type of crystal, it may be verified easily that the same Euler-Poincaré characteristic [4] $\chi = 0$ is valid for the surfaces of both the crystalline torus and the Möbius crystal (*). It would appear that a proof that a crystal may contain dislocations and be « simply connected » has to wait for further developments in lattice topology.

A stringent reason for limiting the crystals under consideration to "simply connected" ones is apparent from figure 3, where the sequence abcd shows that a dislocation in a Möbius crystal may annihilate itself by splitting in two equal dislocations, one of which is caused to change its sign by having traversed the circuit of the Möbius crystal once. And conversely, the sequence dcba demonstrates that a dislocation may be created spontaneously by introducing two dislocations of opposite sign at the same point in the crystal, and having one of these traverse the circuit. The choice of the travelling dislocation determines the sign of the resulting dislocation ! Most evidently, the Burgers vector is not a conservative quantity in Möbius crystals.

Möbius crystals in the extreme forms shown in figure 2 and 3 are not to be commonly expected, as has been remarked by Frank, although they may occur in « pathological crystals like chrysotile ». Nevertheless, the situation remains far from satisfactory, as it is not clear precisely on what principle certain types of crystals should be excluded ; the term « pathological » is not sufficiently precise. Is it really the « connectivity » of the Möbius crystal that makes it a « pathological » case, or does the topological method contain loopholes ?

The question acquires more depth if we consider

(*) The Euler-Poincaré characteristic of a surface is defined as $\chi = V + F - E$, in which : V = the number of vertices, Fthe number of faces and E the number of edges that may be described on the surface. For a cube $\chi = 8 + 6 - 12 = 2$. Topologically, the surface of a sphere is equivalent to that of a cube.



FIG. 3. — The sequence *a-b-c-d* shows that a dislocation in a Möbius crystal may annihilate itself by splitting in two equal components, one of which acquires the opposite sign by traversing the circuit of the crystal.

the dislocations in the crystals shown in figure 4. In the left hand side of the figure a twin crystal is shown. It is assumed that the crystal structure is such that perfect dislocations gliding across the coherent boundary can do so only by leaving behind twinning dislocations. For instance, Sleeswyk and Verbraak [5] have shown that in the b. c. c. lattice $\frac{1}{2}$ [111] disloca-



FIG. 4. — A twin and a bent crystal, which differ only in the crystallographic configuration of their middle parts.

tions gliding across a $(\overline{1}12)$ coherent twin interface will decompose as follows :

$$\frac{1}{2}[111] \to 1/3[111] + 1/6[151]. \tag{1}$$

The Burgers vector 1/6[151] in one twin half is equal to $\frac{1}{2}[111]$ in the orientation of the other half of the twin, while $1/3[1\overline{11}]$ is the Burgers vector of one of the two possible types of $\{112\} < 111 >$ twinning dislocations in b. c. c. If, therefore, the dislocation in the upper half of the crystal glides across the twin boundary, it leaves behind a twinning dislocation schematically shown in the figure — before it may continue on a new glide plane in the lower half.

We now consider the bent crystal, of the same structure, presented in the right hand side of the figure. The bending has been carried out in such a fashion that the orientation of the top half of the crystal is the same as that of the top half of the twin crystal, and that the orientation of the lower halves is also equal. We consider the same glide plane as in the twin crystal; whether or not the bending of the crystal has introduced dislocations is immaterial as long as the dislocations moving on the glide plane do not react with the others, i. e. as long as the other dislocations are not located on the glide plane. This is assumed to be the case. If we now consider a dislocation gliding from top to bottom in the bent crystal, it is evident that according to the current convention no dislocations are produced during the process, in contrast to what happens in the twin.

If the Burgers vector were really a conservative physical quantity pertaining to a dislocation, the passage of the latter from one region of the crystal to another should uniquely be connected with or without production of dislocations independent of the path followed or the crystal structure traversed. Most obviously, this basic requirement is violated in the above example, and unfortunately, it is impossible to have recourse to « pathology » of the crystal, nor is it possible to maintain, for instance, that the twinning dislocation produced by the dislocation passing through the twin boundary is topologically different from a perfect dislocation. If the Burgers conservation law is applicable to Burgers vectors in Euclidean space in the case of the twin, and to Burger vectors defined relative to the curvilinear coordinates presented by the distorted lattice directions in the case of the bent crystal, the apparent contradiction is eliminated, but then the question why two different reference systems should have to be used remains unexplained. That in the present usage the Burgers vector is not rigorously a conservative property, even in « sound » crystals, appears to be the ineluctable conclusion : as will be shown in the following, it is chiefly due to the intuitive topological method used.

Unstable dislocations and the conservation of the Burgers vector. — If we compare the progress of the perfect dislocation in the twin crystal across the twin interface with that of the dislocation in the bent crystal from one unit cell to the next one, there is in fact no basic difference in the initial conditions. The adjoining unit cells in the bent crystal are differently oriented, and so are the unit cells at both sides of the twin boundary : there is only a difference in *degree* of relative disorientation. Apparently disorientation is a necessary but not a sufficient condition for producing dislocations upon the passage of a perfect dislocation through the lattice. It would seem obvious that a second condition is the *stability* of the resulting dislocation.

The twinning dislocation produced in the twin boundary by passage of a perfect dislocation is evidently stable; very small partial dislocations might formally have been produced by the perfect dislocation upon going from unit cell to a neighbouring one possessing a slightly different orientation, if the formalism that a Burgers vector is a vector in Euclidean space is adopted. These very small partials annihilate themselves by elastic deformations : formally, of course, any gradient of elastic deformation in a crystal may be represented by assemblies of very small dislocations, and an elastic deformation can be considered as the movement of such dislocations.

To illustrate the point, and to show in what way a self-consistent model of dislocation movement can be obtained figure 5a may be considered. A small section of a bent crystal is schematically depicted; it is assumed that a dislocation with a Burgers vector which is inclined to the glide plane may glide between the second and the third glide plane, and that the lower part of the crystal is fixed with respect to the reference system, and the upper part mobile. The atoms above the planes between which the dislocation moves will be displaced over a certain distance when the dislocation has passed, i. e. when the influence of the stress field around the dislocation is negligible. Although the Burgers vector, which is identical to the displacement vector on the glide plane, is assumed to be a conservative vector in Euclidean space, it is convenient and entirely permissible to assume that the displacement as transmitted to other planes and cells follows the metric of the distorted lattice. By adopting this convention it is possible to describe a rotation of a portion of the crystal lattice by passage of stable dislocations without being obliged to formally introduce unstable partial dislocations throughout the lattice.

In figure 5*a* the displacement vectors *d* are decomposed in a component d_t tangential to the circle of bending, and a component d_r radial to it. The radial

distance between planes is a constant, and the displacement vectors d_r are all equal to the radial Burgers vector component b_r . If the dislocation that may be associated with this component would glide upwards on the radial glide plane on which it is situated, all radial displacement vector components d_r would be annihilated, and only a tangential Burgers vector b_t and tangential displacement vectors d_t would remain.

If now the stable, perfect dislocation gliding on a bent plane is considered, a similar situation arises if the dislocation goes from one unit cell to the next one. The stability conditions of the lattice are supposed to require that the Burgers vector of the perfect, stable, dislocation remains perpendicular to the radius of curvature of the glide plane. This implies that as the stable dislocation moves, it leaves as unstable partial in each of the unit cells it traverses. The situation is illustrated in figure 5b, where the Burgers vectors of the stable dislocation are shown in the two positions in which the dislocation enters and leaves the crystal. together with the Burgers vectors of the tiny unstable partials left behind in the crystal. The latter may formally annihilate themselves by gliding towards the surface on radial planes in the portion of the lattice that is supposed to be mobile. These Burgers vectors are depicted on a larger scale in the Cremona diagram — well-known in applied mechanics — in figure 5c, in which it is shown that the vector sum of the partials is equal to the vector difference of the



FIG. 5. — Burgers vector in a bent crystal. The assumption that the Burgers vector is a conservative property in Euclidean space leads to the formalism that unstable dislocations are left on the glide plane if a stable dislocation moves on it.

Burgers vectors of the stable dislocation when it enters and leaves the crystal.

In the above two dimensional model it is not difficult to give an expression for the Burgers vector of the partial dislocation that may be left behind by a stable dislocation going from one unit cell to the next one. If the curvature of the dislocation trajectory at a certain point is equal to K, and if the tangential and normal unit vectors at that point are t and n respectively, the derivative of t with respect to the unit length of arc s along the trajectory may be expressed by : dt/ds = Kn. If we consider only dislocations possessing Burgers vectors tangent to the dislocation trajectory, we may express the Burgers vector b as : b = bt. Differentiation gives :

$$\frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}} = \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}}\,\boldsymbol{t} + \boldsymbol{b}\,\frac{\mathrm{d}\boldsymbol{t}}{\mathrm{d}\boldsymbol{s}} = \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}}\,\boldsymbol{t} + \boldsymbol{b}\boldsymbol{K}\boldsymbol{n}\,.$$

The local lattice parameter along the dislocation trajectory is a. If $a \ll 1/K$ and $b \ll 1/K$ the partial that is left behind in a unit cell by the passing stable dislocation has a Burgers vector Δb given by :

$$\Delta \boldsymbol{b} = a \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}} = \frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}} a\boldsymbol{t} + a\boldsymbol{b}K\boldsymbol{n} . \tag{2}$$

In three dimensions the trajectory of a point on the dislocation line may be defined unambiguously by requiring the stable Burgers vector to be everywhere tangent to the trajectory. The trajectory is a threedimensional curve — which in general is *not* a geodesic of the glide plane-of which n, pointing towards the centre of curvature, and the tangent t define the osculating plane [6]. The binormal c is a unit vector defined by $c = t \wedge n$, as shown in figure 6a. The tendency of the curve to leave the osculating plane is expressed quantitatively by the torsion T of the curve. It is defined by db/ds = -Tn. It is possible to define the vector of Darboux D as being composed of :

$$D = Tt + Kc.$$

This vector possesses the property that the derivatives of the unit vectors in the trihedron *ntc*, which are given by the Serret-Frenet expressions, may also be expressed

as the vector product of the unit vector and Darboux vector. Thus : $dt/ds = Kn = D \wedge t$;

$$d\mathbf{n}/ds = T\mathbf{b} - K\mathbf{t} = \mathbf{D} \wedge \mathbf{n};$$

$$d\mathbf{c}/ds = -T\mathbf{n} = \mathbf{D} \wedge \mathbf{b}.$$

The expression for Δb is now :

$$\Delta \boldsymbol{b} = \left(\frac{\mathrm{d}\boldsymbol{b}}{\mathrm{d}\boldsymbol{s}}\right) \boldsymbol{a}\boldsymbol{t} + \boldsymbol{a}\boldsymbol{b}\boldsymbol{D} \wedge \boldsymbol{t} . \tag{3}$$



FIG. 6. — Figure a: trihedron of orthogonal unit vectors ascribed to a spatial curve. Figure b: the composition of the vector of Darboux.

The length of the Burgers vector of a stable dislocation is nearly always a certain fixed fraction of the lattice parameter, so if the latter changes along the dislocation trajectory, $db/ds \neq 0$, and one or more partials will be left if the dislocation follows the trajectory. If the cause of the change in lattice parameter is a stress, the partial dislocations will be quickly annihilated because the lattice simply changes with the stress field. If, on the other hand, the change in lattice parameter is due to the fact that a different crystal lattice lies on the trajectory, the partial may very well be stable. In figure 7 a dislocation is shown in the process of going from a lattice with a lattice parameter a to one with a', and a small partial with a Burgers vector of magnitude (a' - a) is left at the boundary. If the stable dislocation would be followed by more of the same type, the partials left by each of these might coalesce eventually into new mobile dislocations. In other words : the formalism developed



FIG. 7. — The sequence a-b shows a perfect dislocation gliding from crystal lattice with a spacing a into one with spacing a'. A partial dislocation with a Burgers vector of modulus (a'-a) is left at the boundary.

here predicts that if dislocations pass from one crystal lattice to another one, the number of dislocations leaving one crystal is not necessarily equal to the number of dislocations entering the other one. From the point of view of a simple shear model this seems plausible enough, but the topological approach to dislocation theory would not necessarily lead to the same prediction.

Discussion.

If we now first return to the problems that inspired the definition of the Burgers vector as a conservative vector in Euclidean space, viz. the Möbius solid and the bent crystal-twin paradox, it would seem reasonable to request that it would be demonstrated that the original difficulties have been dissipated by the different approach. The twin-bent crystal paradox has in fact already been treated : the Cremona diagram in figure 5c makes it clear that the vector sum of the Burgers vector of the unstable dislocations produced in the bent crystal in figure 4 must be equal to the Burgers vector of the twinning partial left in the twin boundary.

The case of the Möbius crystal given in figure 3 is somewhat more complicated. We may, in order to simplify the discussion, regard this Möbius crystal as being composed of two parts : one part in which the crystal is bent over 360° in the plane containing the central axis, and one portion in which the crystal is twisted around its axis over 180°. If we now consider the stable dislocation passing once through the Möbius crystal, the Cremona diagram of the bent portion is evidently a closed loop of vectors, and the Cremona diagram of the twisted portion consists of a half-loop of vectors describing a helix not lying in the plane of the closed vector loop. The total Cremona diagram of the stable dislocation passing once through the Möbius crystal is presented in figure 8.



FIG. 8. — Cremona diagram of the Burgers vector of the dislocation traversing the circuit of the Möbius crystal in figure 3. The points o, a, b, c and d are lying in the plane which contains the centre-line of the distorted prismatic crystal of which the Möbius crystal was created.

Let oc be the Burgers vector of the dislocation in its original position and oa the Burgers vector in the final position. The original Burgers vector oc is accounted for by the following chain of Burgers vectors consisting of the final stable Burgers vector and the Burgers vectors of the unstable partials :

$$ba-b-c-d-a-e-c$$

The conservation law for Burgers vectors remains valid if the Burgers vector is defined relative to Euclidean space even for « Möbius » crystals.

The method has been used previously by the author [7] in a discussion on tilt walls. These were supposed to result from a hypothetical mechanism in which they would result from reactions between dislocations arriving at the tilt wall from both halves of the bicrystal. The expression for the relation between the tilt angle Θ , the Burgers vector \boldsymbol{b} of the dislocations in the tilt wall, and the spacing d between them, was found to be :

$$b/d = \sin \Theta \tag{4}$$

in contrast to the more widespread expression : $b/d = 2 \sin (\Theta/2)$, which results if a little portion of crystal in an intermediate position is assumed to exist at the tilt wall. The dislocations arriving from both halves of the bi-crystal would glide in this hypothetical region and thus acquire the correct orientation. The

author believes that the method outlined above is more rigorous, and should be employed in all cases where the orientation of the crystal is important.

Finally, it must be remarked that the definition of the Burgers vector can now be given in two ways : there is the physical property of the lattice that the Burgers vector that is a certain fraction of the lattice parameter in a certain direction is stable, there is the geometrically defined local Burgers vector in Euclidean space, having in that system of reference a direction and length that may change in a way prescribed by the stability condition if the dislocation moves to another place in the same lattice, but only by dislocation reactions according to a rigorously applicable Burgers vector conservation law.

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