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INTERACTION OF DISLOCATIONS WITH GRAIN BOUNDARIES

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Résumé.- Les dislocations entrent dans ou partent des joints de grains pendant la déformation et la recristallisation. On suppose que tous les joints de grains peuvent contenir des dislocations. Par conséquent les vecteurs de Burgers sont conservés et les lignes des dislocations ne peuvent que se terminer sur les autres dislocations ou les surfaces.

On traitera donc les phénomènes suivants:

- (1) les sources de dislocations dans les joints de grains,
- (2) le mouvement des dislocations dans un réseau de dislocations,
- (3) la transmission des dislocations à travers des joints,
- (4) l'absorption des dislocations par les joints et "l'étalement du coeur".

On discutera les aspects énergétiques et dynamiques de chaque phénomène et les observations expérimentales.

Abstract.- Dislocations interact with grain boundaries during yielding, creep, and recrystallization. It will be assumed that the dislocation model for grain boundary structure is valid generally. Consequently, Burgers vectors are conserved and dislocation lines can end only on other dislocations or free surfaces.

The following phenomena will be considered:

- (1) grain boundary dislocation sources,
- (2) movement of a dislocation in and through a grain boundary dislocation network,
- (3) transmission of a crystal lattice dislocation across a grain boundary,
- (4) absorption of dislocations and "core spreading".

Energetic and kinetic aspects of each interaction will be discussed and related to experimental observations and grain boundary phenomena.

Introduction

Dislocations interact with grain boundaries during deformation and annealing processes. These interactions are fundamental to the properties of polycrystalline materials. In this paper the following processes which involve dislocation grain boundary interactions will be discussed:

- (a) operation of dislocation sources in grain boundaries;
- (b) movement of a dislocation in and through a network of grain boundary dislocations;
- (c) transmission of a crystal lattice dislocation across a grain boundary;
- (d) absorption of dislocations by grain boundaries.

Wherever possible energetic and kinetic aspects of each interaction will be discussed and related to observations of grain boundary phenomena.

At present there is no consensus regarding a general theory of grain boundary structure. However, the balance of the evidence, which includes electron and x-ray diffraction[1,2], electron microscopy of grain boundary dislocations in a wide variety of materials[3-8], grain rotation experiments[9,10] and computer calculations[11], supports the view that grain boundaries have ordered structures which resist perturbation[12] and are retained even at high temperatures[13] although allotropic transformations may occur. On this basis a grain boundary can be described as an array of dislocations between which specific stable structures are preserved. The interaction of dislocations with grain boundaries then becomes a problem in the properties of dislocation networks. The following rules apply:

- (1) dislocation lines end only on other dislocations or free surfaces.
- (2) Burgers vector and core step height are conserved at nodes.

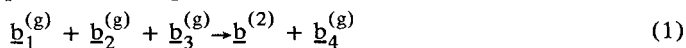
Grain boundary sources of dislocations

Grain boundaries may act as sources of crystal dislocations and grain boundary dislocations. There is *post hoc* evidence for both processes from transmission electron microscopy examination of deformed materials; loops of dislocation are produced presumably by mechanisms rather similar to those by which crystal dislocations are thought to multiply in grain interiors e.g. from sources of the Frank-Read or Bardeen-Herring type[14-16]. Fig. 1 illustrates the operation of a surface source of grain boundary dislocation in copper. Usually the density of grain boundary dislocations is high (of the order $5 \cdot 10^8 \text{ m}^{-2}$; consequently only very short lengths of dislocation may be available to act as sources so that high local stresses are required. The stress to operate a grain boundary source of length ℓ is anticipated to be greater than Gb/ℓ where G is the shear modulus and b is the modulus of the Burgers vector since the multiplication process requires perturbation of the surrounding grain boundary dislocation network.

It is also worth noting that loops of grain boundary dislocation can be produced by aggregation of point defects; this process has been observed in twins[17].

The discussion so far has been concerned principally with the formation of grain boundary dislocations. Grain boundaries may also act as sources of crystal lattice dislocations. Fig. 2 illustrates the generation of lattice dislocations at a grain boundary source in zirconium. Grain boundary steps have been proposed as possible sites for nucleation of lattice dislocations on the basis of stress concentration[18] and observation by transmission electron microscopy[19]. (Murr and associates have made a number of investigations of yielding phenomena by transmission electron microscopy and use the term grain boundary ledge for what is here called a dislocation e.g.[15]).

Study of Li's diagram illustrating the emission of a lattice dislocation from a monatomic step in a grain boundary shows that the process he envisaged[20] may be described as the emission of an absorbed *dislocation* from the grain boundary. It is expected that each dislocation emitted from a grain boundary step would decrease its height by $g \cdot b$ where g is perpendicular to the grain boundary plane and accordingly the source would eventually cease to operate when its stress concentrating effect became too small. It has also been suggested that lattice dislocations might be produced by *association* of grain boundary dislocations[21] essentially by a reversal of the dissociation processes which are discussed later. The concept behind the mechanism is that grain boundary dislocations pile up against some obstacle, a precipitate for example and a reaction such as



occurs in response to the applied stress. (The superscripts designate the structure of which the Burgers vector \underline{b} is characteristic; grain (1), grain (2) or the boundary itself (g). All vectors are referred to the lattice of grain (1)). A difficulty with this kind of process is the likelihood (except in special cases) that one or more of the postulated grain boundary dislocations must move non-conservatively even at low temperatures and high strain rates.

Movement of dislocations in networks

Transmission electron microscopy shows that irregular grain boundary dislocation configurations are characteristic of deformed or recrystallizing material[22,13]. Evidently grain boundary dislocations can move and multiply; *in situ* observations suggest that grain boundary dislocations retain their characteristics at elevated temperatures and whilst grain boundaries are moving. These observations raise significant questions concerning the mechanisms of movement of a dislocation through a dislocation network and the operation of dislocation sources.

An ideal, regular dislocation network is a metastable configuration. In principle a network might move homogeneously but it is more plausible on the basis of fundamental kinetic considerations that some perturbation might propagate through the network in such a way that the final state is equivalent to homogeneous movement but the intermediate steps involve only local rearrangements. This aspect of the structure of dislocation arrays was first investigated in the context of low angle grain boundaries[23,24].

If a regular array of dislocations is regarded as a line lattice an extraneous dislocation appears as a fault in that line lattice. There is a singularity where the extra dislocation enters and leaves the network and a fault, not necessarily stable, where the extra dislocation line interacts with dislocations in the line lattice. Two examples of this behavior are shown in fig. 3. where the extraneous dislocation (a) has and (b) does not have a Burgers vector in common with one member of the network. Movement of the perturbations in the arrays sketched in fig. 3 is equivalent to motion of a dislocation. There is a remarkable correspondence between fig. 3b and a kink on a dislocation line.

The importance of extraneous dislocations to the deformation of networks suggests a possible origin for the well known proportionality between the grain boundary sliding strain and the grain strain during creep[25]. In a sense the same dislocations, albeit with the Burgers vector distribution changed, and similar processes, are responsible for both contributions to the overall deformation. Each dislocation has to pass through the interconnected grain interior and grain boundary networks.

Transmission of crystal lattice dislocations across grain boundaries

Fig. 4 shows the salient features of the crystallography of lattice dislocation transmission across an arbitrary grain boundary. In general a grain boundary dislocation is produced by a reaction of the form:

$$\underline{b}^{(1)} \rightarrow \underline{b}^{(g)} + \underline{b}^{(2)} \quad (2)$$

In order that the dislocation reaction may occur a segment of the incoming dislocation must rotate, at a rate which is generally diffusion limited, from the line of intersection of a slip plane in grain (1) with the boundary into the corresponding line of intersection of a slip plane in grain (2). A dislocation with Burgers vector $\underline{b}^{(2)}$ is then emitted into grain (2), leaving behind a grain boundary dislocation with Burgers vector $\underline{b}^{(g)}$. An alternative and equivalent process would involve the production of the dislocation with Burgers vector $\underline{b}^{(2)}$ from a source in grain (2) followed by a dislocation reaction in the boundary.

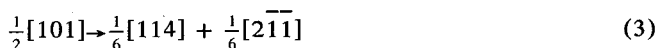
The diffusive transport necessary for reorientation of the incoming lattice dislocation can all take place in the boundary and is short range since adjacent parts of the dislocation are required to climb in *opposite* senses. The stress to expand the loop of $\underline{b}^{(2)}$ dislocation into grain(2) depends inversely on the length of the dislocation which rotates into the correct orientation and the strength of the attractive interaction between the dislocations with Burgers vectors $\underline{b}^{(g)}$ and $\underline{b}^{(2)}$.

The transmission process described above might be expected to occur most readily when slip planes (1) and (2) meet in a common line in the boundary, in which case it has been called "prismatic glide"[26]. For example in fcc metals, at least one set of $\{111\}^{(1)}$ slip planes shares a common line with a set of $\{111\}^{(2)}$ slip planes in tilt boundaries when the rotation axis is of the form $\langle h,k,h + \bar{k} \rangle$. This particular crystallographic arrangement occurs in $\langle 110 \rangle$ tilt boundaries belonging to the $\Sigma=3$ and $\Sigma=9$ (1st and 2nd order twins) coincidence systems; such boundaries are relatively common in fcc metals of medium to low stacking fault energy and silicon[4,27,28].

Since $\underline{b}^{(g)} = \underline{b}^{(1)} - \underline{b}^{(2)}$ it follows, for all coincidence related boundaries, that $\underline{b}^{(g)}$ is a DSC vector (which need not be primitive). The magnitude and direction of $\underline{b}^{(g)}$ can be found graphically, with the help of a coincidence plot or analytically. Both approaches are illustrated by an analysis of some dislocation transmission processes across twin boundaries.

Fig. 5 shows a non-primitive cell of the $\Sigma=3$ coincidence lattice projected onto $(1\bar{1}0)$. It can be seen directly that three of the six $\frac{1}{2}\langle 110 \rangle$ vectors are common to both lattices and the other three pairs of such vectors differ by $\pm \frac{1}{6}[112]$. This means physically that three types of $\frac{1}{2}\langle 110 \rangle$ dislocation may pass across suitably oriented twin boundaries without the creation of any grain boundary dislocations and for the others a $\frac{1}{6}\langle 112 \rangle$ DSC dislocation is left in the boundary.

A reaction of this second type can be written explicitly as follows:



$\frac{1}{6}[114]$ referred to lattice (1) $\equiv \frac{1}{2}[101]$ referred to lattice (2) where the lattices are related by a right handed 60° rotation about $[111]$.

Note that the slip step produced by a dislocation with Burgers vector \underline{b} on a boundary (or surface) normal to the reciprocal lattice vector \underline{g} has a height $\underline{g} \cdot \underline{b}$ planar spacings; for a $\frac{1}{2}[101]$ dislocation and $\underline{g} = 111$, $\underline{g} \cdot \underline{b} = 1$ which is the characteristic core step height of a $\frac{1}{6}\langle 112 \rangle$ DSC dislocation with \underline{b} parallel to the $\{111\}$ twin plane.

Dislocation transmission reactions of the kind described above have been observed and analyzed in $\langle 110 \rangle$ tilt boundaries in copper and stainless steel[26]. It was argued earlier, in the light of the then available evidence that grain boundaries did not act principally as barriers to slip, during low temperature yielding, but mainly as dislocation sources[29]. Evidently both processes are significant.

Absorption of dislocations

Grain boundaries act as sinks for dislocations during primary recrystallization. This behavior may be analyzed in terms of the dissociation of lattice dislocations into grain boundary dislocations with smaller Burgers vectors and the subsequent return of any prior grain boundary dislocation network to equilibrium[30-32]. This equilibration may involve adjustments to the spacing of the original dislocations or energy decreasing dislocation reactions. The actual dislocation dissociations that can occur are governed by the crystallography of the grain boundary concerned. Two or more grain boundary dislocations may be produced by dissociation of a lattice dislocation; the longer the period of the boundary, the smaller are the possible Burgers vectors of the corresponding perfect grain boundary dislocations. (An important exception to this trend is that set of grain boundary dislocation with Burgers vectors approximately parallel to a low index axis of rotation). Consequently the Burgers vectors of the dislocations produced by dissociation can have widely different magnitudes and visibility in the transmission electron microscope. If all the dislocations produced by dissociation have Burgers vectors belonging to the appropriate DSC lattice there is no grain boundary stacking fault created as the grain boundary dislocations separate so that the equilibrium separation is infinity in the absence of other constraints such as interactions with other defects. Another possible dissociation product is a partial grain boundary dislocation. Such dislocations separate domains of grain boundary where the structures are (a) equivalent but formed by a symmetry variant of the relative rigid translation \underline{T} [33] or (b) different and characterized by unrelated values of \underline{T} . In case (b) there is a restoring force opposing the separation of the dissociation products if the alternate structures have different energies.

The possibility of the occurrence of a step at the core of a grain boundary dislocation can affect the products of dislocation dissociation and the topography of grain boundary planes[34,35]. Dislocations with doubly primitive DSC Burgers vectors are predicted to be stable in computer generated models of symmetrical tilt boundaries[36]. Although these dislocations are unstable on a b^2 criterion their core structure, with no step, apparently stabilizes them against dissociation into dislocations with primitive DSC Burgers vectors and core steps. Core energies can strongly affect reactions of finely spaced dislocations where the usually long range elastic fields are cut off at distances comparable with the dislocation spacing.

Just as the Burgers vectors of grain boundary dislocation need not be the shortest possible so also the core step height need not be the minimum possible. A very clear example of the behavior occurs at the nodes of a network of $\frac{1}{6}\langle 112 \rangle$ DSC dislocations for which the minimum core step height is the interplanar spacing, d_{111} , in a $\{111\}$ near twin boundary; one set of dislocations must have a core step of height $2d_{111}$ because of the topographical requirement to conserve core step height at nodes[34].

Usually grain boundary dislocation movement is diffusion limited. The flux necessary for dissociation can always pass along the grain boundary between the two (or more) dissociation products. Essentially, for the case where two dislocations are produced by dissociation lengthening of the part plane corresponding to the component of the Burgers vector normal to the grain boundary of one product and corresponding shortening of that of the other dislocation must occur, fig. 6. The dissociation

$$\frac{1}{2}[101] \rightarrow \frac{1}{10}[310] + \frac{1}{10}[\bar{2}\bar{1}5]. \quad (4)$$

$$\underline{b}^{(1)} \quad \underline{b}_1^{(g)} \quad \underline{b}_3^{(g)}$$

in a $\Sigma=5$ related coincidence boundary on a (210) plane is a specific example of this type of dissociation reaction. Note that the relevant edge components need not be the same. The edge components perpendicular to the boundary with normal reciprocal lattice vector \underline{g} are given by $\underline{g} \cdot \underline{b}^{(1)} = 1$, $\underline{g} \cdot \underline{b}_1^{(g)} = 7/10$ and $\underline{g} \cdot \underline{b}_3^{(g)} = 3/10$. In a special case one of the scalar products for a grain boundary dislocation resulting from dissociation may be zero in which case that dislocation can glide in the boundary.

For the example given this would happen when the boundary plane was (120) or (130). For dissociation of a lattice dislocation into two identical edge dislocations with Burgers vector, b , normal to the grain boundary plane the separation velocity is

$$\frac{dr}{dt} = \frac{DGb\Omega}{2\pi(1-\nu)kTr^2} \quad (5)$$

where D is the grain boundary diffusion coefficient, G the shear modulus Ω the atomic volume, ν Poisson's ratio, k Boltzmann's constant, T the absolute temperature and r the separation. This equation predicts that separations of 100\AA will be reached in times of the order milliseconds at temperatures near $0.5T_m$ [37]. Since 100\AA is comparable with the usual separation of grain boundary dislocations it is expected that the characteristic electron microscope image of a lattice dislocation in a grain boundary will disappear practically instantaneously at recrystallization temperatures.

Sufficient examples of dissociation of a lattice dislocation into grain boundary dislocations have been seen to confirm that this absorption mechanism is correct in boundaries which are near to coincidence orientations. However there is a controversy concerning the generality of the description. The argument hinges on the question whether or not all grain boundaries are ordered. It has been suggested that in certain grain boundaries, those with far from favored structures, the cores of extraneous dislocations "spread" i.e. dissociation into dislocations with infinitesimal Burgers vectors occurs[38-40]. The main experimental evidence in support of this view comes from the observed disappearance, at elevated temperatures, of the images of lattice dislocations which have run into grain boundaries during deformation. Such experiments are seldom done under optimum conditions for resolution of finely spaced dislocation arrays so that the failure to observe grain boundary dislocations does not necessarily imply their absence. In addition the implication of dissociation into infinitesimal dislocations is that the grain boundary energy is insensitive to the relative position of the neighboring grains which is implausible when set against the weight of evidence that grain boundary structures are ordered and qualitatively similar (see introduction). On this basis "core spreading" is more properly described as the dissociation of a lattice dislocation into grain boundary dislocations which are then incorporated into an unresolved network.

Absorption of dislocations can result in a change to the Burgers vector content and hence crystallography of a grain boundary. After cold working, since dislocations are produced as loops, the overall change in Burgers vector density of a grain boundary during recrystallization is small providing boundaries migrate distances comparable with the mean free paths of dislocations. Whilst changes in grain misorientations resulting from dislocation absorption have been observed during creep[41] and subgrain coalescence[42], gross changes in misorientation during recrystallization and grain growth frequently involve twin nucleation, sometimes repeatedly[43,44].

Concluding remarks

The interactions of grain boundaries and dislocations have been considered in the context of an overall continuity as illustrated in Fig. 7. Burgers vector is supposed to be distributed in different quanta, at lattice dislocations and grain boundary dislocations of various kinds, and in varying densities. The reactions discussed here may all be viewed as redistributions of some initial Burgers vector content.

Acknowledgments

I would like to thank Prof. W.A.T. Clark for stimulating discussions during the preparation of this paper, the seminar organizers for the challenge of writing this paper and IBM for the opportunity to think.

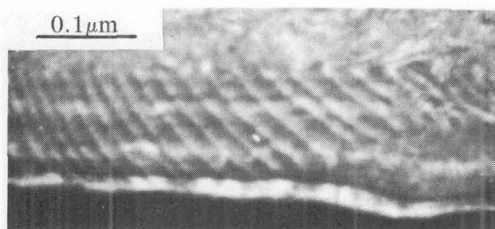


Figure 1

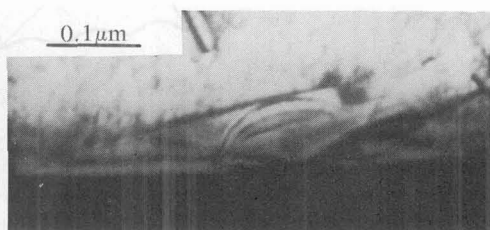


Figure 2

Figure 1 is a transmission electron micrograph showing the operation of a surface source of grain boundary dislocations in copper (courtesy of W.A.T. Clark).

Figure 2 is a transmission electron micrograph showing the operation of a high angle grain boundary source of lattice dislocations in zirconium (specimen courtesy of G.J.C. Carpenter).

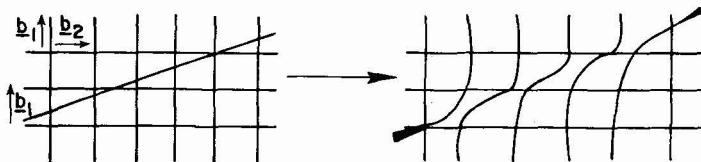


Figure 3a is a sketch showing the perturbations which result in a set of parallel identical dislocations cut by a further dislocation with the same Burgers vector but a different line direction. The perturbations can move along each dislocation line, which process is equivalent to the passage of a dislocation through the original array. Alternatively the perturbations can straighten out which process is equivalent to absorption of an extraneous dislocation.

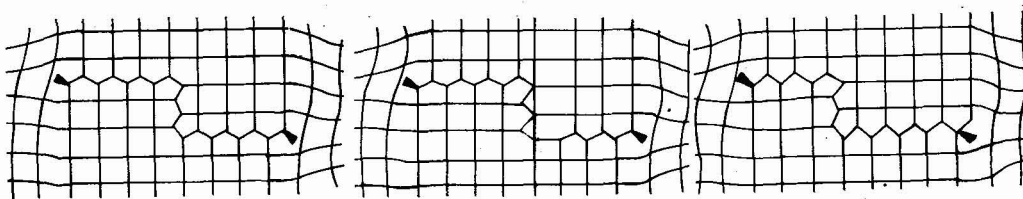


Figure 3b is a series of sketches showing how an extraneous dislocation might move through a square network of grain boundary dislocations by the propagation of a (macroscopic) kink along the extraneous dislocation (after Amelinckx[23]).

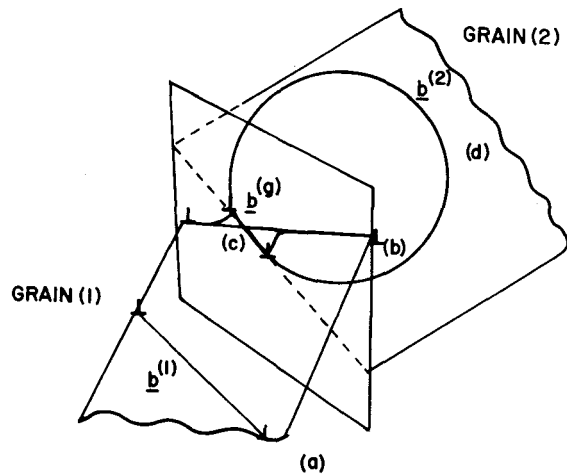


Figure 4 shows schematically the stages in the transmission of a lattice dislocation with Burgers vector $\underline{b}^{(1)}$ across a grain boundary: (a) the dislocation approaches the boundary from grain (1), (b) the dislocation enters the boundary (c) a segment of the dislocation rotates into the correct orientation for glide in grain (2), (d) the segment of dislocation reacts to leave a length of grain boundary dislocation with Burgers vector $\underline{b}^{(g)}$ and a loop with Burgers vector $\underline{b}^{(2)}$ bows out into grain (2).

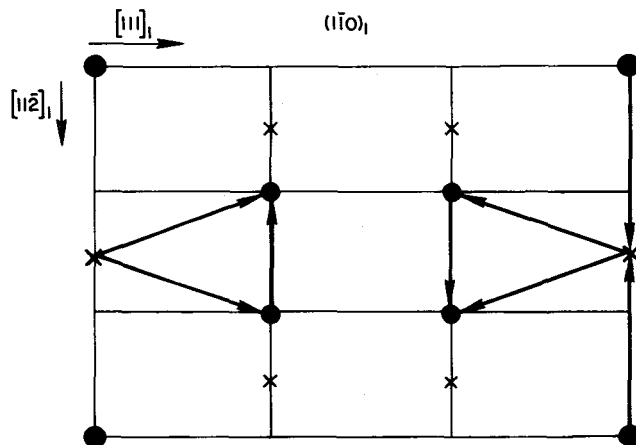


Figure 5 is a $(1\bar{1}0)$ projection of a non-primitive cell of the $\Sigma=3$ coincidence lattice for the fcc case. The bold symbols represent coincidence sites and the dots and crosses designate crystal lattice sites in the distinct (220) layers. The arrows indicate some $\frac{1}{2}\langle 110 \rangle$ Burgers vectors and their shortest differences which are of the form $\frac{1}{6}\langle 112 \rangle$

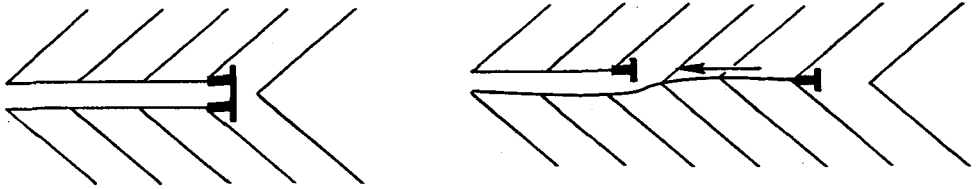


Figure 6 shows schematically how a lattice dislocation may dissociate into two grain boundary dislocations which separate by climb. The arrow indicates the vacancy flux along the grain boundary.

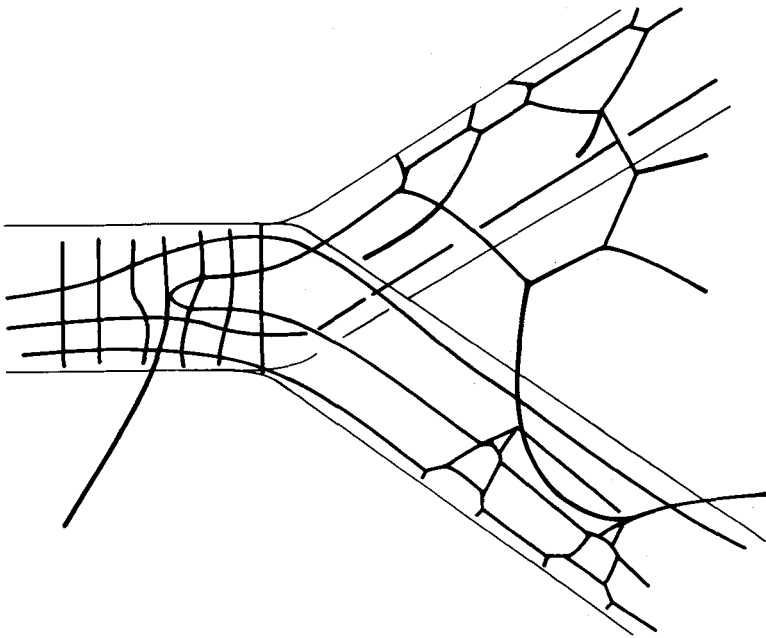


Figure 7 illustrates the continuity of lattice and grain boundary dislocation lines and suggests how dislocation multiplication, absorption and transmission may take place at grain boundaries. Crystal lattice dislocations are shown more lightly than grain boundary dislocations.

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DISCUSSION

J.W. CAHN : Your talk concentrated on moving dislocations interacting with stationary boundaries. We are often faced with moving grain boundaries and such complications as net deposition or removal of atoms by diffusion and lattice parameter differences due to compositioned difference across the boundary. Dislocations must play an important role, but very little attention has been given to even the simplest topological and conservation laws that apply. Can you suggest which of the laws you have given apply, or how they must be modified for these problems?

D.A. SMITH : Providing grain boundaries retain an ordered perturbative resisting structure I would expect dislocation lines to be continuous and Burgers vector and step height to be conserved at nodes as I elaborated in my paper. In that framework deposition or removal of atoms and lattice parameter changes can all be described in terms of dislocation processes, specifically movement and generation of dislocations.

If the boundary structure were to change more drastically than by an increase in point defect concentration, a decrease in solute concentration or an allotropic transformation to another ordered structure, so that the boundary energy was no longer sensitive to the boundary configuration, then I would guess that the idea of a step at the core of a grain boundary dislocation would lose its meaning and Burgers vectors would no longer be discrete; however Burgers vector would still be conserved.

This still leaves unanswered the question of relating the Burgers vector content to the state of a system, if indeed it can be done.

L. HOBBS : You have suggested that rotation of a dislocation segment on the slip plane of one grain to that of the second grain is improbable because it is a non-conservative process. Is this not being a bit unfair? It may require only a cooperative process, like self climbs over short distances. The question is, really, how small must be the new dislocation segment to generate a new loop.

D.A. SMITH : I take your point. Since the stresses at the head of a pile up are so large the local stress can be so high that only a short length, such as 50b, of dislocation needs to reorientate.

- V. VITEK : Transmission of the dislocation through a general grain boundary may not require diffusion in spite of the fact that a component of the Burgers vector perpendicular to the boundary exists. The reason is the multiplicity of structures (see paper by Vitek and Gui Jin Wang) of these boundaries. Movement of the dislocation through the boundary then represents local transformations between different structures which can be easy. However, some boundaries particularly those parallel to low index planes may have low multiplicity and thus may act as strong obstacles to slip.
- D.A. SMITH : Thank you for bringing this interesting possibility to my attention.
- L. PRIESTER : I think that the dissociation reactions are strongly affected by segregation. In the case where segregated species are present before the lattice dislocation impinges the grain boundary, the separation of the products of the dissociation can hardly occur.
- D.A. SMITH : This sounds very reasonable since we expect a strong effect on the climb of dislocations from the presence of impurities. Pinning of grain boundary dislocations, by solute, also provides a mechanism for the solute inhibition of sliding and migration of grain boundaries.