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The Effects on Grain-Boundary Processes of the Steps in the Boundary Plane Associated with the Cores of Grain-Boundary Dislocations

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Abstract

The contribution of the associated steps to the properties of grain-boundary dislocations are investigated. Two methods of step-height determination are given and it is shown that the step height, like the Burgers vector, must be conserved during the reactions of grain-boundary dislocations: this is not always automatic and additional coherent steps must take part in some reactions. The energies associated with steps have been estimated and compared with the elastic energies of grain-boundary dislocations; these comparisons suggest that (*a*) the reduction of elastic energy alone may not be a sufficient criterion for the progress of a reaction and (*b*) that arrays of dislocations may reduce their energy by containing dislocations embodying steps of varying height.

1. Introduction

It has been suggested that grain-boundary dislocations (g.b.d.'s) may be responsible for grain-boundary sliding (Crussard & Tamhankar, 1958), grain-boundary migration (Smith & Rae, 1979) and the absorption or emission of point defects by grain boundaries (Ashby, 1969). The linking of these processes has also been postulated (Pond & Smith, 1976) and it is the purpose of this paper to explore in detail the possible correlations and their consequences.

It is clear that climb and glide of g.b.d.'s must be interdependent in any case where the Burgers vector of a g.b.d. is neither parallel nor perpendicular to the grain-boundary plane, since the motion by pure climb or pure glide of such a dislocation would move it out of the boundary plane. The motion of g.b.d.'s (by glide-plus-climb) may also be linked to boundary migration if steps in the boundary plane are associated with the cores of the g.b.d.'s. Such steps arise in coincidence or off-coincidence boundaries because the grain-boundary structure must remain unchanged by the passage of a g.b.d. if it is perfect, and yet a property of such a g.b.d. is to shift the origin of the coincidence-site lattice (Bollmann, 1970). In general, the only way in which a grain boundary can have the same structure on either side of the g.b.d. is for the boundary plane to move to a different level at the dislocation core.

2. Relationship between g.b.d. and boundary plane

All the correlations between grain-boundary processes which have been proposed are direct results of the relationship between a g.b.d. and the grain-boundary plane in which it lies. For the purposes of this paper, we consider only planar grain boundaries (except where a step is introduced with a g.b.d.) and we further presume that g.b.d.'s can only move in the grain-boundary plane: *i.e.* we assume that the band of stacking faults which would be created by the motion of a g.b.d. away from its boundary plane is of such a high energy in all cases as to prevent such motion.

For convenience in defining grain-boundary planes, we use the vector **n** which lies perpendicular to the boundary plane which it defines and points from grain 1 into grain 2. The Burgers vector of a g.b.d. may be parallel or inclined to the grain boundary plane. It is useful to differentiate three cases:

(i) Where **b** lies perpendicular to **n**. Dislocations of this type may glide in the boundary but cannot climb unless the boundary migrates.

(ii) Where **b** lies parallel or antiparallel to **n**. In this case, the dislocation can climb in the boundary but cannot glide unless the boundary migrates.

(iii) Where **b** lies at an arbitrary angle to **n**. For this configuration the dislocation can move neither by pure glide nor by pure climb, in the absence of boundary migration, since either type of motion will move it away from the grain boundary. This is the most general configuration and such dislocations must move by a glide-plus-climb mechanism.

A g.b.d. with its Burgers vector at an angle φ to the boundary plane may be considered to glide a distance $x \cos \varphi$ and climb a distance $x \sin \varphi$ for every distance x which it moves along the boundary plane. Alternatively, the dislocation may be considered as resolved into inseparable components, $b \cos \varphi$ of which glides and $b \sin \varphi$ of which climbs in the boundary plane.

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Fig. 1 demonstrates the effect of a dislocation in displacing the origin of the coincidence-site lattice (CSL): Fig. 1(*a*) shows four unit cells of the $\Sigma = 5$ (36·9°/[100]) CSL constructed for two f.c.c. lattices. In this system, a DSC lattice vector, any of which is a possible Burgers vector for a perfect g.b.d., is $\mathbf{b} = (a/10)[031]_1$, $(a/10)[03\bar{1}]_2$, where the subscripts refer to the crystal lattice in which the vector is defined. If lattice 2 in Fig. 1(*a*) is displaced by this vector with respect to lattice 1, we achieve the pattern shown in Fig. 1(*b*): the coincidence pattern has been recreated in a different position and for a boundary which was originally at *A* to have the same structure after the displacement of the lattices, it could move to *B*, *C*, *D* or *E*. {The structures on the planes *B* and *D* are identical to those on *C* and *E*, but shifted along the tilt axis by $(a/2)[100]$.}

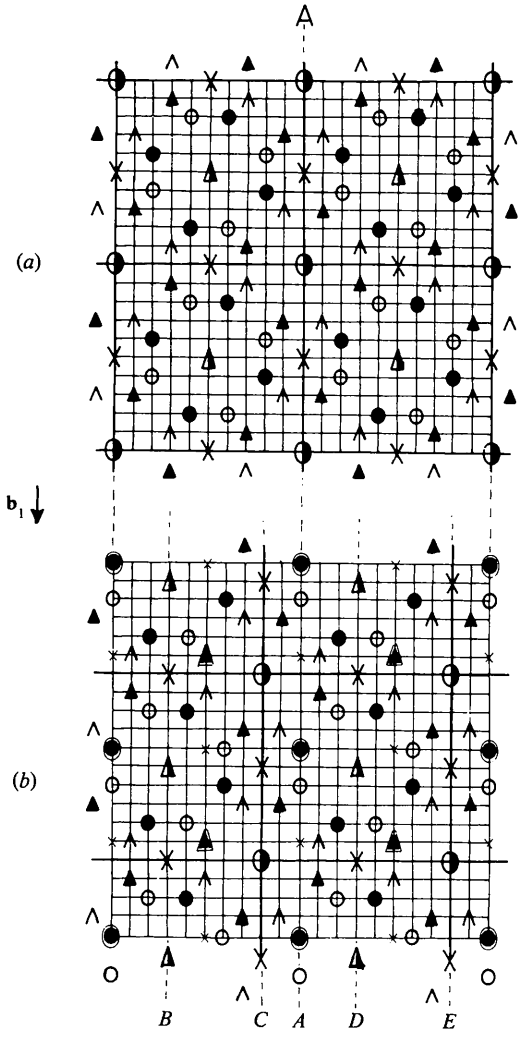


Fig. 1. (*a*) Four unit cells of the CSL for the $\Sigma = 5$ coincidence system in f.c.c. crystals. Filled symbols are lattice 1, unfilled ones lattice 2. The symbols Λ represent sites which are out of the page by $(a/2)[100]$ and the symbols × represent *O*-lattice elements which do not correspond to crystal-lattice sites. (*b*) Obtained from (*a*) by displacing lattice 2 by $\mathbf{b}_1$. Old coincident sites are marked with surrounded symbols and old non-lattice *O*-elements are marked with small crosses.

The sites in Fig. 1 are shown as lattices (*i.e.* fully interpenetrating and extending to infinity): only the sites of lattice 1 are occupied by atoms on one side of the boundary and sites of lattice 2 on the other side, for a real grain boundary. For a pair of semi-infinite grains, there is an infinite number of geometrically equivalent positions for the replaced boundary after displacement of lattice 2 by **b**. They may all be described as the smallest possible movement of the boundary plane plus or minus a coherent step, a coherent step being defined as a step on the grain-boundary plane of height *N* times the CSL periodicity parallel to **n**, where *N* is an integer.

The problem of accurately determining the height of the step associated with a g.b.d. is important in the analysis of any process in which grain-boundary dislocations are thought to play a role. Two methods will be given: geometrical construction and calculation following Pond (1977), which is extended and generalized here.

2.1. *Step height by construction*

Consider again Fig. 1. We can construct a vector from an old coincidence site to a new one. This will be called a step vector, **s**. By convention, lattice 1 is kept stationary while lattice 2 is displaced by **b**. In this case the step vector is measured with respect to lattice 1 and is called $\mathbf{s}^{(1)}$. It is physically equivalent to keep lattice 2 stationary while displacing lattice 1 by $-\mathbf{b}$. In this case, **s** measured with respect to lattice 2 is $\mathbf{s}^{(2)}$. The step vectors are related by

$$\mathbf{s}^{(1)} = \mathbf{s}^{(2)} + \mathbf{b}. \tag{1}$$

This is illustrated in Fig. 2. There is an infinite number of choices of the step vector in either reference lattice, but they are all related by the addition of CSL vectors **c**: we may therefore arbitrarily choose the shortest step vector, $\mathbf{s}^{(\alpha)'}$, where α is either 1 or 2. Any step vector is then given by

$$\mathbf{s}^{(\alpha)} = \mathbf{s}^{(\alpha)'} + \mathbf{c}. \tag{2}$$

The height of the step associated with the dislocation is now simply

$$h_\alpha = \mathbf{s}^{(\alpha)} . \mathbf{n}_\alpha. \tag{3}$$

The shortest step vector does not necessarily give the smallest step height. Also, the step height as measured in lattice 2 differs from the step height as measured in lattice 1 since

$$\begin{aligned} h_1 &= \mathbf{s}^{(1)} . \mathbf{n}_1 \\ h_2 &= (\mathbf{s}^{(2)} - \mathbf{b}) . \mathbf{n}_2. \end{aligned} \tag{4}$$

The difference in step heights as measured with respect to lattices 1 and 2 is thus

$$\Delta h = \mathbf{b}.\mathbf{n}, \tag{5}$$

i.e. the climb component of the Burgers vector: this is a reasonable result, since, if we resolve the Burgers vector of an edge dislocation parallel and perpendicular to the grain-boundary plane, we essentially have two half-planes of extra material, one of which represents the climb component of the dislocation and lies parallel to the boundary plane. This extra material may be associated with either grain 1 or grain 2, which therefore has a step on its surface equal to the height of the step on the other grain plus the thickness of the layer of extra material, which is $\mathbf{b}.\mathbf{n}$. The difference in step heights is thus a real effect which would be manifested by cutting a bicrystal containing a g.b.d. along the boundary plane: the surfaces thus revealed would have stress-free steps of height h_1 on crystal 1 and h_2 on crystal 2.

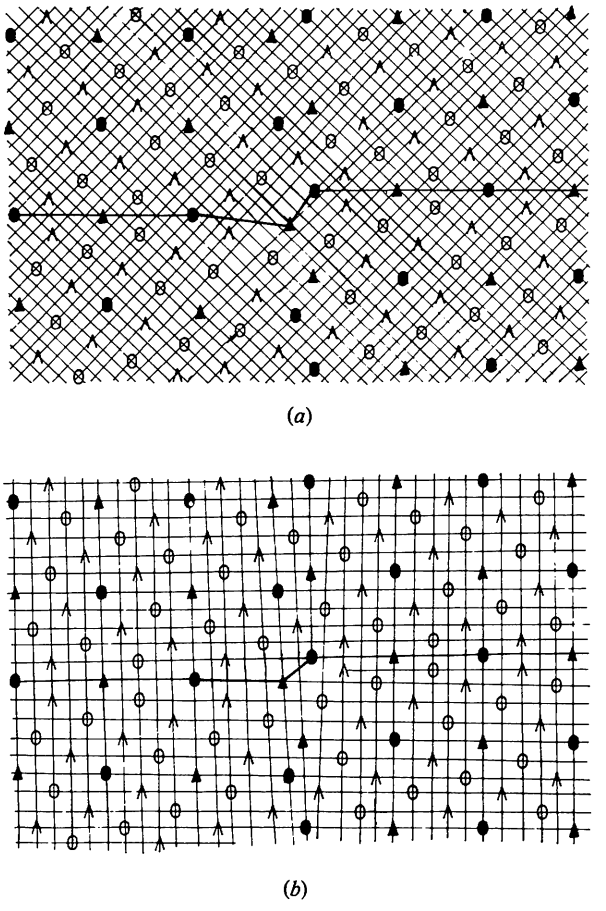
As an example, consider Fig. 3 which shows a dislocation of Burgers vector $(a/10)[0\bar{1}3]_1$ in a $\Sigma = 5$ grain boundary lying on a $(012)_1(021)_2$ plane passing through coincidence sites. The choice of a plane passing through coincidence sites gives us a useful reference state—it does not imply that atoms actually occupy coincidence sites—and a translation away from this position, provided it was conserved on either side of the dislocation, would not change the result of the analysis.

The step vectors used in the construction of Fig. 3 are

$$\mathbf{s}^{(1)} = \frac{a}{2}[110]_1,$$

$$\mathbf{s}^{(2)} = \frac{a}{2}[110]_2.$$

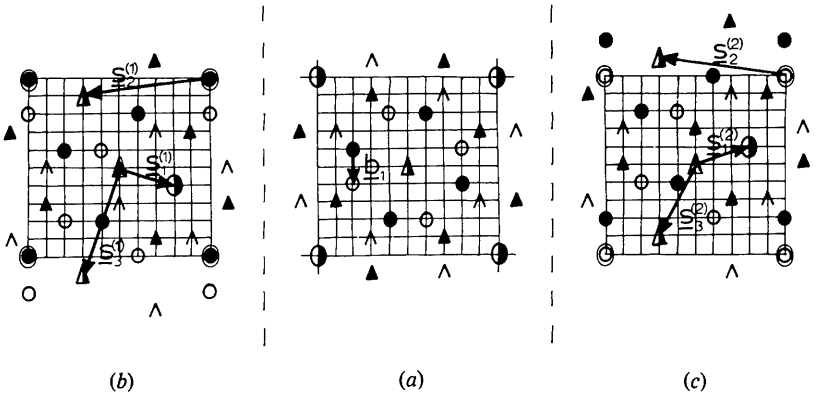
These are the vectors which join the first and last coincidence sites on either side of the g.b.d., in the boundary plane. In order to get the step height as a number of planes parallel to the grain boundary, we define $\mathbf{n}$ as the reciprocal-lattice vector corresponding



(*a*)

(*b*)

Fig. 3. Two pictures of the same dislocation: (*a*) with DSC lattice lines drawn in to emphasize the extra half-plane; (*b*) with lines drawn parallel and perpendicular to the boundary plane to emphasize the step. (Coincident lattice sites are filled.)



(*b*) (*a*) (*c*)

Fig. 2. Construction of step vectors, $\mathbf{s}^{(1)}$ and $\mathbf{s}^{(2)}$ in the $\Sigma = 5$ system: (*b*) is obtained from (*a*) by displacing lattice 2 by $\mathbf{b}_1$; (*c*) is obtained from (*a*) by displacing lattice 1 by $-\mathbf{b}_1$.

to the lattice planes parallel to the boundary. Thus,

$$\mathbf{n}_1 = [024]_1,$$
$$\mathbf{n}_2 = [042]_2,$$

which gives

$$h_1 = 1\ (024)_1 \text{ plane},$$
$$h_2 = 2\ (042)_2 \text{ planes}.$$

These steps are clearly seen in Fig. 3(*b*) where planes are drawn parallel and perpendicular to the grain boundary to emphasize the steps and illustrate that the difference in step height is indeed the climb component of the g.b.d.

In cases where the boundary plane is parallel to a rational plane of the CSL, many of the step vectors give rise to identical step heights: for example, in Fig. 2, $\mathbf{s}_1$ and $\mathbf{s}_3$ give the same step height for a boundary lying on the $(012)_1(021)_2$ plane.

Bollmann's (1970) work on shifts of the coincidence pattern is in terms of the *O* lattice, rather than the CSL: the *O* lattice takes in coincidences between non-lattice sites of identical internal coordinate as well as coincident lattice sites. The use of step vectors joining old and new *O*-lattice elements does not generally give the correct answer for the step, although under special circumstances it will do so: this only occurs when the boundary plane under consideration lies parallel to planes which run through coincident lattice sites and non-coincident site *O*-lattice elements without a step. In the $\Sigma = 5$ example given above, this condition is fulfilled, for example, for the $(031)_1$, $(0\bar{1}3)_1$ and (100) planes; in other cases the step height found by the *O*-lattice technique is half of that found by the CSL technique, because there is always a plane of non-coincident site *O*-elements between each pair of planes containing coincident sites. The *O*-lattice technique does not distinguish between the two types of *O* element, and stepping from a plane containing one type to a plane containing the other will cause a change in structure.

2.2. *Step height by calculation (in-plane translation analysis)*

Pond (1977) has given a method for finding the possible step heights by calculation, utilizing an approach different from that outlined above, but which was only developed for the case where **b** lies in the boundary plane. For this case, Pond found

$$\mathbf{b}_i^L = \mathbf{b} + n\,\mathbf{m}_1, \tag{6}$$

where $\mathbf{b}_i^L$ is a lattice vector lying in the boundary plane, **b** is the Burgers vector of the dislocation under consideration, $\mathbf{m}_1$ is an in-plane translation vector equivalent to displacing the boundary plane by one layer and n is the number of layers parallel to the boundary which the step comprises. By allowing all possible in-plane lattice vectors, we get all the possible step heights. When he developed this technique, Pond (1977) stated that for Burgers vectors perpendicular to the boundary plane, the extra material could, in principle, be accommodated by symmetrical relaxation. This is only true, however, when the extra material exists as an even number of crystallographic half-planes, such as in the $\Sigma = 5$ case where a Burgers vector of $(a/10)[310]$ comprises two (620) half-planes. In cases where there is an odd number of half-planes, we must create an asymmetrical step. The in-plane translation analysis for this case will be illustrated by reference to the $\Sigma = 11$ coincidence system which is created in cubic lattices by a rotation of 50·48° about a common [110] axis. A possible Burgers vector in a f.c.c. $\Sigma = 11$ grain boundary is $(a/11)[1\bar{1}3]_1$ and Fig. 4

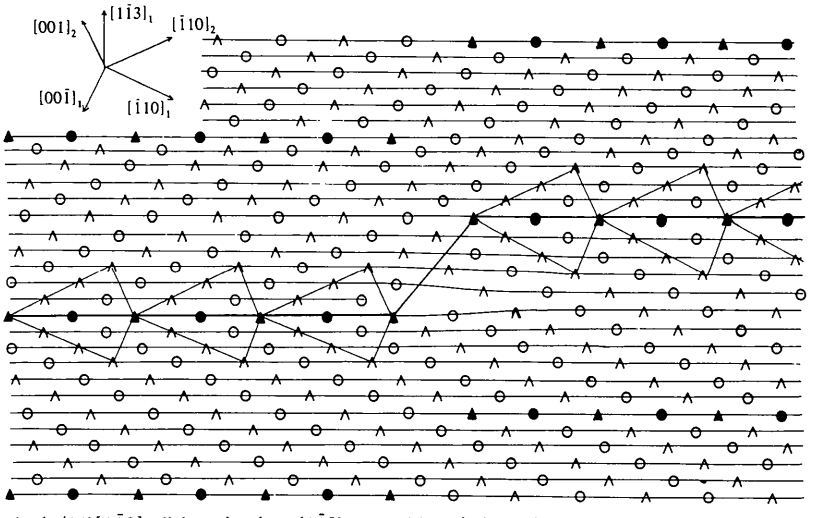


Fig. 4. $(a/11)[1\bar{1}3]_1$ dislocation in a $(1\bar{1}3)_1$, $\Sigma = 11$ grain boundary between two f.c.c. crystals.

shows this dislocation in a $(1\bar{1}3)_1$ boundary at the coincidence position. The dislocation comprises one extra $(1\bar{1}3)_1$ half-plane.

The effect of inserting the extra half-plane of atoms just above the boundary plane (in grain 2) is to translate the rest of crystal 2 to the right by $\mathbf{i}_2$ (following Pond's notation). This translation is analogous to the translation due to the Burgers vector of the g.b.d. in the in-plane Burgers vector case, so we can write

$$\mathbf{b}_i^L = \mathbf{i}_2 + n\,\mathbf{m}_2. \tag{7}$$

For the example shown, $\mathbf{i}_2 = (a/22)[\bar{9}9\bar{6}]$, $\mathbf{m}_2 = (a/11)[996]$ and $\mathbf{b}_i^L = (a/2)[\bar{3}3\bar{2}]$ which gives $n = 5 \pm 11N$. The $\pm 11N$, where N is an integer, accounts for other geometrically correct possibilities allowed by considering integer multiples of $\mathbf{b}_i^L$. Note that n is the number of planes by which the boundary is displaced in addition to the inserted extra half-plane, so the total is $6 \pm 11N$ for crystal 2 and $5 \pm 11N$ for crystal 1. The difference in step heights is, in this case, the Burgers vector of the g.b.d.

We now have two techniques for determining the possible step heights associated with g.b.d.'s: they are different in approach but both yield the same result if correctly applied. The techniques are compared from the point of view of the user in Table 1.

We can now generalize to some extent about the nature of the step which may be associated with the various types of g.b.d. which were described above. For this purpose we are concerned with the stress-free steps which would be revealed by cutting a bicrystal along the boundary plane. The possible step forms are:

1. No step on either crystal.
2. Equal step on each crystal (g.b.d. motion displaces the boundary plane).
3. Equal but opposite step on each crystal (g.b.d. motion does not displace the boundary plane, but moves grain centres toward or away from each other).
4. Unequal steps on each crystal (g.b.d. motion displaces the boundary plane and grain centres have a component of motion toward or away from each other).

4*a*. As 4 but one of the crystals has no step.

The step forms and dislocation natures which may be associated with the various types of dislocation are summarized in Table 2.

Step form 1 is a special case which may be associated with some variants of step form 2 as step forms 3 and 4*a* are special cases of step form 4. A step of form 1 is always transformed to a step of form 2 by the addition of a coherent step and forms 3 and 4*a* are always transformed to 4 by the same process.

Table 1. *Comparison of the two techniques for finding step heights associated with g.b.d.'s*

CSL construction	In-plane translation
Demands knowledge of entire CSL unit cell. (May be awkward for large values of Σ.)	Demands knowledge of entire boundary-plane periodicity. (May be awkward for high-index planes, even for low Σ.)
May be readily applied to any g.b. plane once step vectors found.	Specific to boundary plane: must be recalculated if plane changes.
Specific to Burgers vector: must be reconstructed for new **b**.	May be readily applied to any Burgers vector on a specific plane.
One-step process for any angle between **b** and **n**.	Two-step process for general angles between **b** and **n**.
Can be adapted for non-rational planes.	Works only for rational planes.

Table 2. *Step forms and dislocation natures which may be associated with various types of g.b.d.*

G.b.d. description	Step forms allowed	Dislocation natures
b parallel to **n**	3, 4, 4*a*	Edge
b perpendicular to **n**	1, 2	Edge, mixed, screw
b at angle to **n**	4, 4*a*	Edge, mixed

3. Reactions of grain-boundary dislocations

Grain-boundary dislocations have many of the properties of crystal-lattice dislocations and some of the rules governing their reactions can be inferred directly from those for crystal-lattice dislocations, *e.g.* the conservation of Burgers vector. In addition to the condition that the Burgers vector is conserved at a dislocation node, in grain boundaries we have the additional condition that the total step in the boundary plane must be conserved: this is illustrated in Fig. 5 and can be proved by use of the in-plane translation analysis. Consider two dislocations with Burgers vectors $\mathbf{b}_a$ and $\mathbf{b}_b$, and for convenience have them both lying in the boundary plane, so (6) applies:

$$\mathbf{b}_{ia}^L = \mathbf{b}_a + n_a\,\mathbf{m}_1, \tag{i}$$

$$\mathbf{b}_{ib}^L = \mathbf{b}_b + n_b\,\mathbf{m}_1. \tag{ii}$$

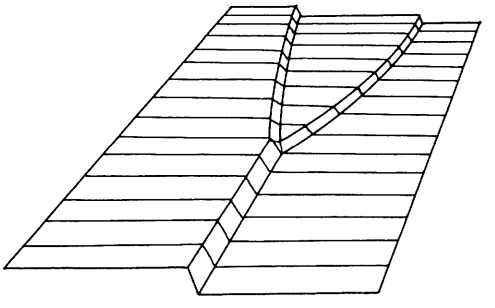


Fig. 5. Schematic illustration to show that steps on the grain-boundary plane must be conserved for topographical reasons.

If the two dislocations react together forming the Burgers vector $\mathbf{b}_s$, then adding (i) to (ii) describes this product in terms of its Burgers vector and step:

$$\mathbf{b}_a + \mathbf{b}_b = \mathbf{b}_s$$

and from (i) and (ii)

$$\mathbf{b}_{ia}^L + \mathbf{b}_{ib}^L = \mathbf{b}_s + (n_a + n_b)\,\mathbf{m}_1,$$

so the total step in the boundary plane is still $(n_a + n_b)$ layers parallel to the boundary, although if n_a and n_b represented the minimum step heights for $\mathbf{b}_a$ and $\mathbf{b}_b$, $(n_a + n_b)$ need not necessarily represent a minimum step height for $\mathbf{b}_s$.

Pond & Smith (1977) have considered the absorption of crystal-lattice dislocations by grain boundaries in terms of dissociation into primitive DSC dislocations. This provides a useful framework for some examples to illustrate the step conservation principle. It is first necessary to establish the nature of the step created on the boundary plane by a run-in, undissociated lattice dislocation. This is most conveniently achieved by the following thought experiment (Fig. 6). Take a bicrystal containing a planar grain boundary and separate the two crystals (Fig. 6*b*). Run a dislocation into the boundary plane from one crystal: this introduces a slip step on the crystal surface of height $\mathbf{b}.\mathbf{n}$; no step is created on the other crystal, although the crystallographic planes parallel to the boundary may be elastically buckled. This is in agreement with (5) and inspection of the illustration of a run-in dislocation in Pond & Smith (1977) also confirms the hypothesis.

We can now investigate, in terms of step heights, the dissociations of two different lattice dislocations in a $\Sigma = 5$ grain boundary. The dissociations, in the coordinate system of crystal 1, are

$$\frac{a}{2}[011] = \frac{a}{10}[0\bar{1}3] + \frac{a}{10}[031] + \frac{a}{10}[03\bar{1}], \quad (A)$$

$$\frac{a}{2}[0\bar{1}1] = \frac{a}{10}[0\bar{1}3] + \frac{a}{10}[0\bar{1}3] + \frac{a}{10}[03\bar{1}] \quad (B)$$

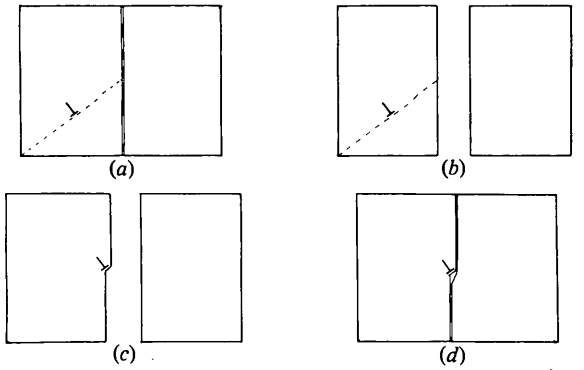


Fig. 6. Thought experiment to determine the step heights associated with a run-in crystal-lattice dislocation.

and we shall consider the (012) boundary plane, so $\mathbf{n} = [024]$. The step vectors and step heights for the various dislocations used in this example are given in Table 3. Now, if we rewrite the two reactions in terms of step heights, assuming that the smallest possible step is the most stable configuration for each g.b.d., we get

$$3 = -1 + 2 + 2, \quad (A)$$

$$1 \neq -1 - 1 - 2. \quad (B)$$

This means that dissociation *A* will give only the three product dislocations with their smallest possible steps, but dissocation *B* must either give a step of +4 (024) layers to one of the $(a/10)[0\bar{1}3]$ dislocations, a step of +3 (024) layers to the $(a/10)[03\bar{1}]$ dislocation or an additional step of 5 (024) layers, equal to the CSL periodicity perpendicular to the grain boundary. Performing the analysis with crystal 2 as the reference frame gives the same result, showing that the step-height calculations are self-consistent.

The possibility of the formation of additional coherent steps on a grain boundary by crystal-lattice dislocation absorption may be important in calculations of the velocity of a dislocation along a grain boundary, since a dislocation which moves mainly by glide on a particular boundary plane may have to move mainly by climb to pass such a step: this could constitute a rate-limiting process for the motion of such a dislocation. If a population of dislocations was being forced into a boundary during the course of a deformation experiment, this would give a mechanism for the progressive increase in the sliding resistance of the boundary in addition to that derived from elastic interactions between g.b.d.'s and lattice dislocation pile-ups.

4. Energetics of g.b.d. reactions

In the previous section, a new constraint on the possibility of a g.b.d. reaction has been demonstrated. The

Table 3. *Step vectors and heights for the various dislocations considered in the crystal-lattice dislocation dissociation examples*

Burgers vector	$\mathbf{s}^{(1)\prime}$	$\mathbf{s}^{(2)\prime}$	$\mathbf{h}_1(024)_1$ planes	$\mathbf{h}_2(042)_2$ planes
$\frac{a}{2}[011]_1$	use $\mathbf{b}$	Nil	3	0
$\frac{a}{2}[0\bar{1}1]_1$	use $\mathbf{b}$	Nil	1	0
$\frac{a}{10}[0\bar{1}3]_1$	$\frac{a}{2}[1\bar{1}0]_1$	$\frac{a}{2}[1\bar{1}0]_2$	$-1 \pm 5N$	$-2 \pm 5N$
$\frac{a}{10}[031]_1$	$\frac{a}{2}[101]_1$	$\frac{a}{2}[101]_2$	$2 \pm 5N$	$1 \pm 5N$
$\frac{a}{10}[03\bar{1}]_1$	$\frac{a}{2}[\bar{1}01]_1$	$\frac{a}{2}[\bar{1}0\bar{1}]_2$	$-2 \pm 5N$	$-1 \pm 5N$

direction in which a reaction will proceed is determined as the direction of lowering of free energy. For crystal-lattice dislocations, this is usually reduced to the Frank b^2 criterion which assumes that the energy of each dislocation is proportional to b^2, and ignores core-energy terms and energies of interaction between the dislocations. There is a further approximation in the case of grain-boundary dislocations, since no step-energy terms are considered either.

For the two examples given in the previous section, the b^2 criterion predicts a 40% energy reduction in both cases. If we assume that step energy is proportional to step height, as suggested by Pond & Smith (1977), then we get a 40% reduction in step energy going in the opposite direction for dissocation A and an 86% saving for reaction B {assuming that the additional coherent step is associated with one of the $(a/10)[0\bar{1}3]$ dislocations}. Clearly, the direction in which the reaction will proceed depends on the relative sizes of the step energy and the elastic energy of the dislocations. Atomistic calculations, such as those performed by Vitek, Sutton, Smith & Pond (1979) do not provide a means of separating step, core and elastic energy terms for a dislocation, so it is worthwhile to consider estimates made from rather simpler arguments.

Pond & Smith (1977) have assumed that the step energy is equal to the increase in grain-boundary area due to the step times the grain-boundary energy which was assumed to be isotropic. Furthermore, they assumed that the step would be right-angled. We can now investigate the effects of removing these two assumptions by considering a step such as in Fig. 7. The energy of the sloping face of the step is γ' and that of the principal boundary plane is γ; a unit length of step will be considered. The energy saving due to the loss of area of the principal boundary plane is $\gamma h/\tan\rho$ and the loss due to the area of the sloping face of the step is $\gamma' h/\sin\rho$, so the total step energy is

$$E_s = h\left(\frac{\gamma'}{\sin\rho} - \frac{\gamma}{\tan\rho}\right). \qquad (8)$$

Fig. 8 shows how this energy varies, per unit step height, as a function of ρ for various values of the ratio $\gamma':\gamma$. For a real grain boundary, this ratio would also vary with the angle ρ, but the values shown give an indication of the order of magnitude of the step energy.

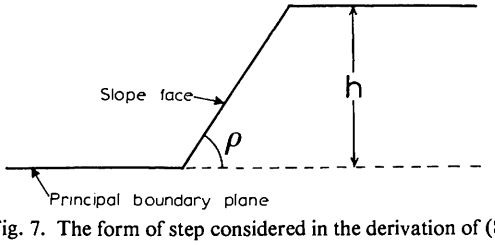


Fig. 7. The form of step considered in the derivation of (8).

Taking into account variations of the ratio $\gamma':\gamma$ with ρ may lead to a curve of E *vs* ρ which displays different minima from those shown for constant values of the ratio: these will correspond to favoured step configurations for the dislocation and boundary under consideration.

A further energy contribution owing to the existence of a step at each g.b.d. core arises for dislocations which form an array, since these will be prevented, if they have edge character, from attaining their lowest energy configuration, Fig. 9. The interaction energy for a pair of like edge dislocations at a fixed separation has a minimum when the angle α (Fig. 9*b*) is $\pi/2$. The force on the upper dislocation in a direction perpendicular to the line joining the two dislocations is

$$F_\alpha = \frac{\mu b^2}{2\pi(1-\nu)}\frac{\sin 2\alpha}{r}. \qquad (9)$$

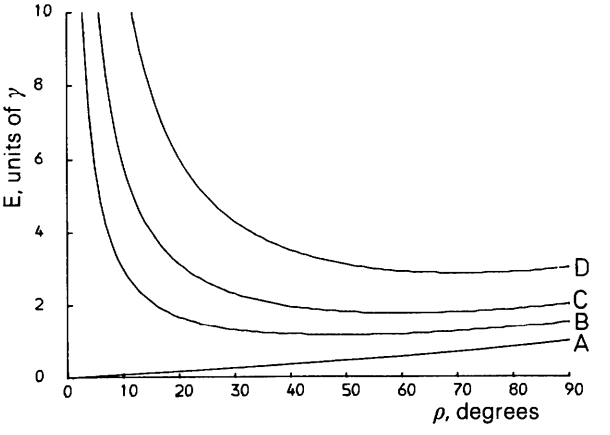


Fig. 8. Energy of a unit length of step of unit height, in units of γ, for varying step inclination and slope-face energy. The ratios of slope-face energy to principal boundary-plane energy are (*A*) 1; (*B*) 1·5; (*C*) 2; (*D*) 3.

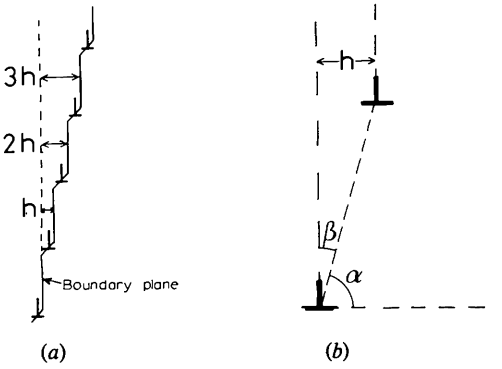


Fig. 9. (*a*) Steps at dislocation cores prevent the g.b.d.'s from achieving their minimum-energy configuration in an array. (*b*) Definition of h, α and β for finding the energy associated with such a displacement.

The work done against this force in removing the upper dislocation from its minimum-energy position to some other value of α is

$$E_{s(A)} = \frac{\mu b^2}{2\pi(1-\nu)} \int_{\pi}^{\alpha} \frac{\sin 2\alpha}{r} \, d\alpha \qquad (10)$$

$$= \frac{\mu b^2}{4\pi(1-\nu)} \frac{\cos 2\alpha}{r}$$

$$= \frac{\mu b^2}{4\pi(1-\nu)} \frac{\sin 2\beta}{r}. \qquad (11)$$

If β is a small angle (step height is small compared with dislocation separation), we can substitute $2h/r$ for sin 2β, giving

$$E_{s(A)} \simeq \frac{\mu b^2 h}{2\pi(1-\nu) r^2}. \qquad (12)$$

Now if the dislocation was at the centre of an infinite array, this energy would be increased to take account of interactions with all the other dislocations in the array and

$$E_{s(A)} = \frac{\mu b^2 h}{2\pi(1-\nu) r^2} \sum_{-\infty}^{\infty} \frac{1}{n^2}, \qquad (13)$$

which is equal to

$$E_{s(A)} = \frac{\pi \mu b^2 h}{6(1-\nu) r^2}. \qquad (14)$$

This is the energy associated with the step at the core of the central dislocation in the array: it is only correct if all the dislocations have identical steps and if **b** lies parallel to **n**; for other cases, the step energy may be more, less or negative. In particular, a lower-energy structure may be produced by a mixture of step heights giving an average, taken over all the dislocations in the array, of zero.

The elastic energy of a dislocation with inner cut-off r_i and outer cut-off r_o is

$$E_e = \frac{\mu b^2}{4\pi(1-\nu)} [\ln(r_o/r_i) - 1] \qquad (15)$$

and the extent of the strain field of a dislocation in an array is roughly equal to the array spacing (Van der Merwe, 1950), so substituting r for r_o in (15) gives an estimate of the elastic energy of a dislocation in an array. It can now be seen that the contribution of step energy increases as the array spacing decreases, and the elastic energy decreases. Thus, for small dislocation spacings in arrays, the step energy becomes increasingly important in determining the direction in which a dislocation reaction will proceed, and Frank's b^2 criterion becomes correspondingly unreliable.

As an extreme example for dislocations not belonging to arrays, consider again Fig. 4: the dislocation in this case may have a step of +5 or −6 $(1\bar{1}3)_1$ layers (as measured in grain 1) and has a Burgers vector of $(a/11)[1\bar{1}3]_1$. A possible step form for a dislocation with twice this Burgers vector is a type 3 step, Fig. 10. For step-energy calculations, it is convenient to use an effective step height which may be defined as the average of the step heights measured with respect to grains 1 and 2, so a type 3 step for example has an effective height of zero. We can now write the reaction

$$\frac{2a}{11}[1\bar{1}3] = \frac{a}{11}[1\bar{1}3] + \frac{a}{11}[1\bar{1}3]$$

and in Al the effective steps are

$$0 \qquad +6{\cdot}71 \qquad -6{\cdot}71 \text{ Å}.$$

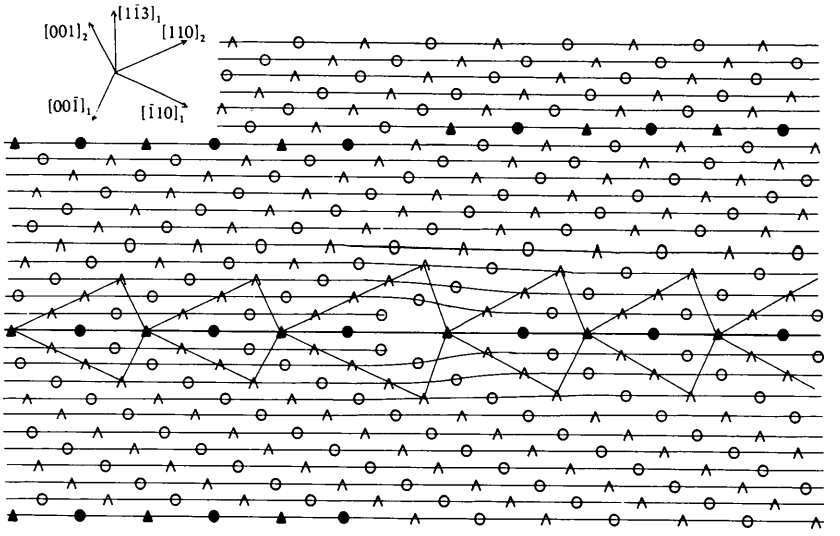


Fig. 10. $(2a/11)[1\bar{1}3]_1$ dislocation in a $(1\bar{1}3)_1$, $\Sigma = 11$ grain boundary between two f.c.c. crystals.

From (15), with inner cut-off 5, outer cut-off 1000 Å and constants appropriate to Al, the energy balance for the reaction comes out as

$$8{\cdot}05 \times 10^{-10} \Rightarrow 2{\cdot}02 \times 10^{-10} + 2{\cdot}02 \times 10^{-10}\ \mathrm{J\ m^{-1}}.$$

Now, with an isotropic form of (8) and a typical value for the grain-boundary energy of Al, 0·625 J m^{-2} (Inman & Tipler, 1963), and with the trigonometrical term equal to 0·5, the step-energy balance is

$$0 \Leftarrow 2{\cdot}20 \times 10^{-10} + 2{\cdot}20 \times 10^{-10}$$

and adding the two energy balances gives

$$8{\cdot}05 \times 10^{-10} \Leftarrow 4{\cdot}22 \times 10^{-10} + 4{\cdot}22 \times 10^{-10}\ \mathrm{J\ m^{-1}},$$

i.e. the reaction will proceed in the direction of association, even though the b^2 criterion predicts a dissociation. The energy difference is, however, very small and in view of the approximations made, no great reliance can be placed on this prediction, which is used here merely to suggest how marginal the energy balance may be for a g.b.d. reaction, since step energies and elastic energies for these dislocations may be of the same order of magnitude.

5. Discussion

The fact that it may be energetically favourable or even crystallographically necessary for dislocations of identical Burgers vector to embody different steps is new, and may have interesting consequences. The motion of g.b.d.'s is accompanied by shuffles of atoms across the boundary plane, when the g.b.d. has an associated step (see, for example, King & Smith, 1979), and the number of such shuffles is related to the step height. It is possible that this effect will increase the Peierls stress for motion of g.b.d.'s by glide, and thus dislocations of identical Burgers vector may respond differently to an applied stress if they have different steps.

The experimental measurement of step heights on the scale necessary to distinguish between the various possibilities or a g.b.d. is extremely difficult, but might be achieved by means of lattice-imaging transmission electron microscopy: we look forward to some interesting results from this new field of experimentation. Effects such as differing mobilities may, however, be more easily observed in conventional transmission electron microscopy with *in situ* experiments.

6. Conclusions

(i) Two methods of step-height calculation have been given: possible step heights are related to the coincidence geometry of the bicrystal, but not simply to the angle of the Burgers vector to the boundary plane.
(ii) The necessity for step-height conservation has been demonstrated for g.b.d. reactions, and it has been shown that minimum step heights are not always maintained for all the dislocations involved in a reaction.
(iii) The energies associated with g.b.d. core steps have been estimated and it has been shown that: (*a*) an array of dislocations may lower its energy by containing dislocations of differing step height; (*b*) Frank's b^2 criterion may be unreliable for g.b.d. reactions.

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