Grain-boundary shear-migration coupling. II. Geometrical model for general boundaries

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Received 18 December 2008; received in revised form 13 January 2009; accepted 13 January 2009
Available online 18 March 2009

Abstract

Grain boundary-mediated plasticity is now a well-established phenomenon, especially in fine-grained or nanocrystalline metals. It has been described in several models, but most of these apply to very exclusive configurations such as symmetrical grain boundaries, or grain boundaries that possess a specific coincidence orientation relationship. In real polycrystals, grain boundaries have random orientations, and the current models cannot account for the shear associated with their migration (see part I of this study [1]). The present work presents a model of shear-migration coupling in which grain boundaries do not have specific orientation relationships. It consists in defining couples of shear and rotation values, able to transform one lattice orientation into another, regardless of the type of boundary that separate them. This purely geometrical model can be seen as a generalized formulation of the existing shear coupling theories. No long-range diffusion is involved, but very localized atomic shuffling is generally necessary in the core of mobile interfacial dislocations.

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Keywords: Grain boundary migration; Dislocations; Plastic deformation; Modelling

1. Introduction

First studied in bicrystals [2–6], the phenomenon of stress-induced grain boundary (GB) migration has recently seen renewed interest because it appears as a likely alternative plasticity mechanism in very small-grained and nanograined metals [7–13]. In particular, those recent observations were carried out at ambient or low temperature [7,14], suggesting that a process such as Coble creep is not involved. These experiments have raised a number of questions concerning the basic mechanisms responsible for GB motion and shear-migration coupling: is it stress driven? Does it imply diffusion? What is the shear produced by a moving GB? What are the pertinent crystallographic parameters to predict this shear?

Sorting out the causes of GB motion has proved difficult in complex materials such as nanocrystals where the initial structure may be rich or poor in dislocations depending on the processing route. Recrystallization has long been known as a process in which high-angle GBs move under the stored strain energy accumulated during heavy deformation [15]. In dislocation depleted or relaxed nanocrystalline films, GB motion has, however, clearly been attributed to stress concentration [10,16]. Extensive bicrystal experiments also showed that the velocity of a given GB was a linear function of the applied stress [17,18].

Answering the second question is also crucial since diffusion-based processes, also called “non-conservative” (Coble creep, diffusion-induced grain boundary migration (DIGM)), may not produce any systematic shear. On the other hand, “conservative” models of GB migration do not involve any diffusion and could theoretically operate at any temperature, including room temperature and below. To date, only two conservative models predicting a finite number of shear values are available and will be discussed extensively in the present work: the Cahn–Taylor–Mishin model [19,20], hereafter called “Cahn’s model”, and the DSC (displacement shift complete) model [21–24].
The experimental basis for this study was developed in the part I of this work and consists in transmission electron microscopy in situ straining experiments performed in ultrafine-grained (UFG) Al [1]. Indeed, nanograin materials contain a large fraction of random boundaries, but are too small to allow detailed investigations. We have assumed that the underlying mechanisms are the same in UFG and nanograin Al because GB motion exhibits several common aspects in both materials. A recent in situ study also points to similar GB motion behavior both in the nanograined (<100 nm) and UFG (>100 nm) regimes [10], giving a basis for the present assumption.

The experiments described in part I show that the application of an external stress considerably enhances GB migration and that the migration mechanism is coupled with a shear displacement parallel to the boundary plane, as in bicrystals [1]. There are thus strong indications of similar behaviors, in bicrystals and in polycrystals, on one hand, and in polycrystals and nanograin materials, on the other. The available dislocation-based models, which can account for the properties of bicrystals with coincidence misorientation relationships and pure tilt symmetrically controlled boundaries [25,26], cannot, however, be used in polycrystals, where boundaries have random misorientations and planes, and where there are many compatibility constraints at triple junctions. This also calls for a more general description of shear-migration coupling, which could apply to a large variety of non-crystallographic interface planes and non-coincidence misorientations.

Such a new model is proposed in this second part. The model is purely geometrical but does allow very local diffusion, as in the theory proposed by Babcock and Balluffi (thereafter called the “shuffling model”) where atoms may shuffle with a magnitude that is smaller than nearest-neighbor atomic spacing [4]. Because it involves only very short-range rearrangement, this model is conservative, and can be confronted to Cahn’s and DSC models. After a brief description and comparison of the available conservative models in Section 2, the new model is described in Section 3, and several consequences for the behavior of polycrystals are evoked in Section 4.

2. Available models of conservative GB migration

2.1. Shuffling with no coupled shear

The shuffling mechanism was first proposed by Rae [27], who observed the fast motion of high-angle boundaries in Al, associated with a negligible lateral motion of the visible DSC dislocations. The author accordingly described the migration in terms of “atom jumps” across the interface. Similar observations of moving Σ5 boundaries in gold were subsequently made by Babcock and Balluffi [4]. For the same reason, and since no plastic deformation could be measured after migration, the DSC dislocation mechanism was rejected, and the boundary migration was ascribed to the reorganization of the atomic structure inside each unit cell of the coincidence site lattice (CSL), with no average shear displacement.

In contrast to the DSC dislocation model, and since no interfacial dislocation glide motion is involved, the shuffling mechanism should a priori work for any boundary plane, provided the misorientation exhibits a high degree of coincidence (low Σ). A closely related process has been observed in atomistic simulations by Zhang and Srolovitz [28], and Schonfelder et al. [29]. In both cases, the boundary motion was activated by an external biaxial stress inducing different elastic energies in both half crystals. It is important to note that this type of solicitation, which exists only in anisotropic media, induces no permanent plastic deformation. In Al, this should result in the growth of grains with <100> “soft” directions parallel to the biaxial stress directions.

2.2. Motion of dislocations with DSC Burgers vectors

Grain boundary migration resulting from the stress-induced motion of DSC dislocations has been proposed by Rae and Smith [24], and by Guillope and Poirier [6], to account for experimental results in Cu, Al and NaCl. The so-called coupling factor can be expressed by the ratio β = s/m, where s is the amount of shear parallel to the interface plane, and m is the corresponding migration distance. The shear s is proportional to the length of the DSC Burgers vector involved, and the migration distance m is proportional to the corresponding step height h, which depends on the position of the Burgers vector in the elementary cell of the CSL. This model will be discussed in more details in Section 3.2, as a particular case of the general model. Geometrical restrictions inherent to this process are the following:

(i) The misorientation must exhibit a high degree of coincidence (low Σ).

(ii) In case of a conservative process, the boundary plane must be parallel to the Burgers vector of the gliding DSC dislocations. This implies that boundaries are parallel to a low-index direction of the DSC and CSL lattices. Pure tilt boundaries are accordingly most often—but not always—symmetrical.

This mechanism has been observed in several bicrystals verifying the above conditions: in NaCl [6], Al [30], Zn [31] and cubic zirconia [32]. The non-conservative process involving the climb motion of DSC dislocations has also been observed in Au bicrystals [5]. The migration of Σ5 symmetrical tilt boundaries controlled by the glide motion of DSC dislocations has been reproduced by atomistic calculations in body-centered cubic (bcc) iron [33].

2.3. Cahn’s model [19,20,34]

In this recent approach, high-angle boundaries are described as an array of of edge dislocations with Burgers
vector perpendicular to the boundary plane, similarly to low-angle GBs. Since only one dislocation family is required, the description is restricted to symmetrical tilt boundaries. The Burgers vectors can be parallel to either $<100>$ or $<110>$ directions, which yields the two distinct "mode 1" and "mode 2" mechanisms. This model will be described in more detail in Section 3.2, as a particular case of the general model. Its different requirements and domain of validity can be summarized as follows:

(i) The boundary must be symmetrical, with a pure tilt character.
(ii) In case of a low-$\Sigma$ coincidence orientation relationship (OR), the boundary motion can alternatively be described by the DSC dislocation mechanism [19].
(iii) The extension of the model to non-symmetrical boundaries should be possible, although difficult [19]. Indeed, the boundary must then be described by a mixture of dislocations with various Burgers vectors, gliding in intersecting planes, and crossing each other during migration.

This model has been validated by atomistic simulations (only in case of low-$\Sigma$ misorientations, however [19,34]), and by experiments in $11^\circ$-misoriented bicrystals [35]. The amount of shear produced by the Cahn model is of the order of several tens of percent, i.e. definitely larger than that observed in strained polycrystals (part I).

2.4. Comparison of available models

The three models of conservative boundary motion described above exhibit several analogies and differences which can be summarized as follows:

(i) In all cases, the migration involves the reorganization of the atomic structure inside a small volume. In the shuffling mechanism, this volume has a fixed shape (i.e. corresponding to the CSL unit cell), which yields no deformation. In the DSC dislocation mechanism, the reorganization takes place in a volume sheared in the direction of the Burgers vector, which yields some plastic deformation. In this respect, the shuffling mechanism can be considered as a particular case of the DSC dislocation mechanism, where the Burgers vector of the DSC dislocations is zero. The atomic reorganization occurring in the Cahn mechanism has been described in detail only in the case of $\Sigma 17$ and $\Sigma 37$ boundaries [36]. In this case, it should be similar to that of the equivalent DSC dislocation mechanism. An alternative description of the DSC dislocation mechanism in terms of pure shuffling (as in the shuffling model) plus glide of a tilt boundary of DSC dislocations (in the same way as in the Cahn model, except that DSC dislocations are considered instead of perfect ones) has been presented in Ref. [37].

(ii) According to atomistic simulations, the applied stress has a twofold effect corresponding to two different driving forces: producing a permanent plastic deformation in the DSC and Cahn models, and producing no permanent deformation in the shuffling model. As a result of this difference, the elastic strains included in the shuffling model favor the growth of grains with specific orientations with respect to the applied stress, whereas the plastic shear of both other models has a priori no clear effect on the final texture. Note, however, that the elastic strain energy may also be included in the models of shear–migration coupling, with the same consequences as in the pure shuffling model, although this effect has been considered negligible by Gianola et al. [8].

(iii) The models of migration-induced shear are restricted to either coincidence boundaries in low-index planes (DSC dislocations), or symmetrical boundaries (Cahn). This seems insufficient to account for the stress-induced motion of boundaries in a polycrystal, where grain boundaries have random misorientations and habit planes, and where the direction and intensity of shear produced at a given boundary must be compatible with those produced at adjacent ones.

(iv) The amounts of deformation predicted are very different from each other: zero for the shuffling model, very large (several tens of percent) for the Cahn model, intermediate to very large for the DSC dislocation model.

In conclusion, the application field of the available models appears too restrictive to account for the experimental results described in the first part of this study [1]. Indeed, the conservative motions of random grain boundaries in polycrystals, as well as the compatibility of the deformation of adjacent grains, require a very large spectrum of shear possibilities which are not provided by these models. It is thus necessary to give a more general description of shear–migration coupling, valid for a large variety of GB planes and misorientations. Such a model is proposed in what follows, and we will see that it gives rise to a larger number of shear values for a given misorientation between two grains.

3. Geometrical model of conservative stress-induced GB motion

3.1. Methods

This general model is valid for a large variety of non-coincidence and asymmetrical tilt GBs, and yields various shear–migration coupling factors. It is purely geometrical and based on the unique condition that a local reorganization of small groups of atoms, with no long-range diffusion (atomic shuffling), is possible during the migration process. This reorganization is described in the planes perpendicular to the rotation axis between two grains, assumed to be
dense planes. In order to realize this condition, we tile these planes with motifs which, in the most general case, are parallelograms with atoms at their corners (Fig. 1).

Let us consider as an example the tiling of the \{110\} planes of the face-centered cubic (fcc) structure. Two parallelograms with the same area ("a" and "b"), enclosing the same number of atoms, are shown in Fig. 1a and b. This ensures that the transformation of one parallelogram into the other is conservative. Fig. 1c and d shows that their external shapes can be transformed into each other by a rotation of angle \(\varphi\), followed by a shear deformation (dashed arrows). This means that a group of atoms (Fig. 1e) can change its shape by pure shear (Fig. 1f), provided the lattice is locally rotated by the angle \(\varphi\). This shear deformation represents what can be retrieved when the lattice is forced to rotate by the angle \(\varphi\), which occurs when the GB migrates under stress. In what follows, \(\varphi\) will thus be the rotation angle across a grain boundary. This procedure is generalized by (i) defining families of parallelograms enclosing the same number of atoms, and (ii) determining the rotations and shear deformation connecting each pair of a given family.

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Fig. 1. Description of the method used to determine shear–migration coupling mechanisms for general boundaries. (a and b) Selection of two parallelograms containing the same number of atoms. (c and d) Transformation of a into b, by a rotation of angle \(\varphi\), and a shear. (e and f) Transformation of a group of atoms into another one by the same shear, accommodated by a shuffling rotating the lattice by the same angle \(\varphi\).
To determine a family of parallelograms enclosing the same number of atoms, we first define two orthonormal axes \( x \) and \( y \), parallel to dense rows (which is usually possible in cubic crystals), and with unit vectors of length equal to \( 1/2\langle 110\rangle \) (the smallest interatomic distance in the fcc structure). We then consider one or several rectangles with sides defined by vectors \( u \) and \( v \) (respectively parallel to \( x \) and \( y \): Fig. 2a), and the same surface \( uv \). We then

Fig. 2. General method to determine a family of parallelograms with same area. Here, each parallelogram encloses eight atoms in a \( \{011\} \) plane. In this plane, the interatomic distances, normalized by the cubic parameter, are \( \sqrt{2} \) along the horizontal axis (\( \langle 100 \rangle \) direction) and 1 along the vertical axis (\( \langle 011 \rangle \) direction).
perform a series of shear deformations, first along \( x \), and then along \( y \), thus transforming the rectangles into parallelograms. Only small shear amplitudes are considered, in order to select parallelograms with closely related shapes.

The first shear is noted \( p \) (Fig. 2b) because it moves the upper side by a distance \( p \) along the (horizontal) \( x \) axis. Of course, \( p \) must be a multiple of the interatomic distance along \( x \). The second shear is noted \( q \) (Fig. 2c), and displaces the right side along the (vertical) \( y \) axis. After these two successive shears, the vector \( \mathbf{u} = (u, 0) \) is transformed into \( \mathbf{u}' = (u, q) \), and the vector \( \mathbf{v} = (0, v) \) is transformed into \( \mathbf{v}' = (u, v + r) \), where \( r = pq/u \). The ratio \( r \) must be integer, to ensure that each new corner falls on an atomic position.

Each parallelogram with sides \( \mathbf{u}' \) and \( \mathbf{v}' \) is noted \((u, v, p, q)\). The examples shown in Fig. 2, in a \( \{110\} \) plane, correspond to \( u = 8\sqrt{2} \) \( (u = 2\sqrt{2} \) and \( v = 4 \) (Fig. 2a–e) or \( u = \sqrt{2} \) and \( v = 8 \) (Fig. 2f and g)). The parallelograms defined in Fig. 2d and e, are those used as an example in Fig. 1.

Referring to Fig. 1, the parameters describing the rotation \( \phi \), and the associated shear to proceed from one parallelogram \((\mathbf{u}', \mathbf{v}') = (u_a, v_a, p_a, q_a)\) to another one \((\mathbf{u}_b, \mathbf{v}_b) = (u_b, v_b, p_b, q_b)\), are now determined.

A shear deformation is characterized by the shear factor, \( \beta \) (see Section 2.2), and by two undistorted directions along which the distances are unchanged (Fig. 3). As seen in Fig. 3, the first undistorted direction (hereafter called “\( \text{ud}_1 \)”) is the invariant direction parallel to the shear direction, whereas the second one rocks from the direction \( \text{ud}_2a \) to the direction \( \text{ud}_2b \), symmetrical to \( \text{ud}_2a \) with respect to the normal to \( \text{ud}_1 \). The rocking angle, \( \pi - 2\alpha \), is such that the shear factor is

\[
\beta = 2 \tan(\pi/2 - \alpha)
\]

For a given couple of parallelograms \((\mathbf{u}_a', \mathbf{v}_a')\) and \((\mathbf{u}_b', \mathbf{v}_b')\), there are \( 2 \times 2 \) rotations, and associated shear deformations, which can bring them into coincidence (Fig. 4). Two transformations connect \( \mathbf{u}_a' \) to \( \mathbf{u}_a' \) and \( \mathbf{v}_a' \) to \( \mathbf{v}_a' \), and two others ones connect \( \mathbf{u}_b' \) to \( \mathbf{v}_b' \) and \( \mathbf{v}_b' \) to \( \mathbf{u}_b' \). They are illustrated in Fig. 4a–d and e–h, respectively, in the case of the transformation between the parallelograms defined in Fig. 2d and e, also represented in Fig. 1. The two transformations connecting \( \mathbf{u}_a' \) to \( \mathbf{u}_b' \), and \( \mathbf{v}_a' \) to \( \mathbf{v}_b' \), have the same pair of undistorted directions, the same shear factor \( \beta \), but different rotation angles \( \phi \). Each rotation brings one pair of undistorted directions parallel to each other, in such
a way that the subsequent shear is parallel to this direction (i.e. the two parallel undistorted directions correspond to the invariant direction). The roles of both undistorted directions are thus exchanged between both transformations (Fig. 4a–d). The two other transformations, connecting \( \mathbf{u}_a \) to \( \mathbf{v}_a \) and \( \mathbf{v}_a \) to \( \mathbf{u}_a \), are shown in Fig. 4e–h. They generally yield rather large values of \( \beta \), in the most frequent cases where the lengths \( \mathbf{u}_b \) and \( \mathbf{v}_b \) are close to the lengths of \( \mathbf{u}_a \) and \( \mathbf{v}_a \), respectively.

In order to completely characterize this transformation, the key point is thus the determination of the two pairs of undistorted directions.

Let us consider the transformation of a parallelogram \((u_a, v_a, p_a, q_a)\), with sides \( \mathbf{u}_a \) and \( \mathbf{v}_a \), into another one \((u_b, v_b, p_b, q_b)\), with sides \( \mathbf{u}_b \) and \( \mathbf{v}_b \). The direction parallel to a vector \( \mathbf{u} + x\mathbf{v} \) is undistorted when \( \mathbf{u}_a' + x\mathbf{v}_a' \) and \( \mathbf{u}_b' + x\mathbf{v}_b' \) have the same length, namely when:

\[
(u_a + xp_a)^2 + (q_a + x(v_a + r_a))^2 = (u_b + xp_b)^2 + (q_b + x(v_b + r_b))^2
\]

This occurs for two values of \( x \):

\[
x_1, x_2 = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A}
\]

where \( A, B \) and \( C \) are integers defined by:

\[
A = p_a^2 - p_b^2 + (v_a + r_a)^2 - (v_b + r_b)^2
\]

\[
B = 2[u_mp_a - u_mp_b + q_d(v_a + r_a) - q_b(v_b + r_b)]
\]

\[
C = u_a^2 - u_b^2 + q_a^2 - q_b^2
\]

The slopes of the two undistorted directions in the first parallelogram, \( u_{d1a} \) and \( u_{d2a} \), are thus:

\[
P_{1a} = \frac{q_a + x_1(v_a + r_a)}{u_a + x_1p_a} \quad (7)
\]

\[
P_{2a} = \frac{q_a + x_2(v_a + r_a)}{u_a + x_2p_a} \quad (8)
\]

In the second parallelogram, the slopes of \( u_{d1b} \) and \( u_{d2b} \) are:

\[
P_{1b} = \frac{q_a + x_1(v_b + r_b)}{u_b + x_1p_b} \quad (9)
\]

\[
P_{2b} = \frac{q_a + x_2(v_b + r_b)}{u_b + x_2p_b} \quad (10)
\]

The first step to transform parallelogram \((u_a', v_a') = (u_1, v_1, p_a, q_a)\) into \((u_b', v_b') = (u_0, v_0, p_b, q_b)\) is to make two possible rotations, so as to bring the two first or the two second pairs of undistorted directions respectively parallel to each other. These rotations are thus:

\[
\phi_1 = \tan^{-1} P_{1b} - \tan^{-1} P_{1a},
\]

for \( u_{d1a}/u_{d1b} \) (common direction named \( u_{d1} \)), and

\[
\phi_2 = \tan^{-1} P_{2b} - \tan^{-1} P_{2a},
\]

for \( u_{d2a}/u_{d2b} \) (common direction named \( u_{d2} \)).

After rotation, both parallelograms shown in Figs. 2 and 4 can now be transformed into each other by a pure shear of amplitude \( \beta = 2 \tan(\pi/2 - x) = 2/\tan x \) (Eq. (1)), where \( x \) is the angle between the two undistorted directions of slopes \( P_{1a} \) and \( P_{2a} \) (or equivalently \( P_{1b} \) and \( P_{2b} \)) (see Fig. 3). This yields:

\[
\beta = 2 \frac{1 + P_{1a}P_{2a}}{P_{1a} - P_{2a}} = 2 \frac{1 + P_{1b}P_{2b}}{P_{1b} - P_{2b}}.
\]

An important particular case arises when the undistorted directions are dense rows of both crystals, which occurs when \( x \) is integer (slopes equal to rational entities multiplied by the ratio of the interatomic distances along \( y \) and \( x \)), namely when \( \sqrt{B^2 - 4AC} \) is integer. In this case, the rotations \( \phi \) between the two grains connect dense rows with equivalent atomic spacing, which corresponds to coincidence ORs. This particular case is treated first, because it corresponds to situations already described by the DSC dislocation model. The more interesting general case will be described in Section 3.3.

3.2. Coincidence orientation relationships

Coincidence ORs are obtained when both undistorted directions are low-index dense rows, namely when the discriminant \( \sqrt{B^2 - 4AC} \) is integer. In practice, since this square root is difficult to estimate a priori, coincidence ORs can be directly obtained by choosing pairs of parallelograms with either a common side (e.g. Fig. 2a,b and a,c) or a common diagonal (Fig. 2a and f). Under such conditions, one undistorted direction is along this common low-index direction, and the second one will coincide with another low-index direction. It is easy to check that \( \sqrt{B^2 - 4AC} \) is actually integer for all these situations, because \( C = 0 \) for the \((2\sqrt{2}/4,0,0)\) and \((2\sqrt{2}/4, -2/0)\) couple of Fig. 2a and b, and because \( A = 0 \) for the \((2\sqrt{2}/4,0,0)\) and \((2\sqrt{2}/4,0,-1)\) couple of Fig. 2a and c.

For the couple of parallelograms \((2\sqrt{2}/4,0,0)\) and \((2\sqrt{2}/4,0)\) in Fig. 2a and f, which can alternatively be generated by a shear parallel to the diagonal of the rectangle (Fig. 5), we have \( \sqrt{B^2 - 4AC} = 8 \). The corresponding
migration mechanisms are depicted in Fig. 6. In this figure, the initial lattice is represented by open circles, plain or dashed. It is transformed by the migration of the GB (taken along $u_d_1$ in Fig. 6a and $u_d_2$ in Fig. 6b). The GB is pure tilt if perpendicular to the figure plane, and mixed in the alternative case (see Section 4). The transformed lattice is represented by grey circles. The rotation $u_1$ yields the $R_3$ coincidence, and the corresponding boundary plane is along the shear direction, i.e. parallel to the undistorted direction $u_d_1$ (Fig. 6a). The rotation $u_2$ yields the $S_11$ coincidence, and the corresponding boundary plane is along $u_d_2$ (Fig. 6b). The roles of each undistorted direction are exchanged between both solutions, and the common coupling factor is $b = 0.354$.

Fig. 6 shows that the migration of the boundary, to the left in Fig. 6a, and to the bottom in Fig. 6b, can result in the shear transformation of the rectangles ($2\sqrt{2}, 4, 0, 0$), into the parallelograms ($\sqrt{2}, 8, -\sqrt{2}, 0$), as the rotation occurs. This can alternatively be described by the glide of DSC dislocations (also called disconnections), of Burgers vector $b$, associated with steps of height $h = b/h$, to the bottom-right in Fig. 6a, and to the left in Fig. 6b. The number of atoms involved in an elementary displacement of the disconnection is 4 (grey area), i.e. twice lower than the number of atoms embedded in the parallelograms. This happens because the motifs chosen are twice larger than the smallest possible ones, which are ($2\sqrt{2}, -\sqrt{2}, 0$) and ($\sqrt{2}, 4, -\sqrt{2}, 2$).

Fig. 6 also shows that other coupling factors could be obtained with the same $S_3$ and $S_11$ ORs, and same boundary planes, e.g. by the motion of DSC dislocations with Burgers vectors $b_{(\text{Cahn})}$. These two alternative mechanisms correspond to the so-called modes 1 and 2 of the Cahn mechanism, for which the undistorted directions rocking during the migration are respectively $<100>$ and $<110>$.

These modes 1 and 2 are in fact obtained each time one undistorted direction is taken parallel to $<100>$ or $<110>$. This situation is described in Fig. 7, for a rotation around a $<100>$ axis, and for an interface parallel to a $<310>$ direction. Both couples of parallelograms shown in Fig. 7a and b have been constructed with one undistorted direction ($u_d_1$) along $<310>$, and the other ($u_d_2$) along $<110>$, in Fig. 7a, and $<100>$, in Fig. 7b. The corresponding transformations are (1,1,0,0) to (1,1,1,0), and (2,6,0,0) to (2,6,5,2). Fig. 7c and d shows that they generate both modes 1 and 2, with the same $S_3$ OR. The corresponding disconnections have Burgers vectors $b$, and step heights $h$.

3.3. General case

In the general case, the rotations $\varphi$ yield no coincidence OR, and the habit plane of the GB, parallel to the shear direction, is irrational in both crystals. Fig. 8a shows the migration–shear coupling for a rotation around a $<100>$ axis, and for the couple of parallelograms (4,5,0,−1) and (4,5,−1,0). As in the preceding case, the habit plane of the GB goes through undistorted directions defining invariant directions.

Fig. 8b and c shows that the motion of the irrational boundary interface can be treated using the topological model of Pond et al. [22], originally derived to describe martensitic transformations. Both half crystals are first constrained, (i) in order to impose coincidence along two parallel dense rows, e.g. in A, B, C, and (ii) in order to

Fig. 6. Shear–migration coupling in the particular case of a coincidence ORs in a (011) plane. The original lattice corresponding to the shrinking grain is represented by white discs (plain and dashed) while the transformed lattice corresponding to the extending grain is represented by grey discs. Coinciding atoms are circled: the misorientation is of $S_3$ type in (a), and $S_11$ type in (b). The boundaries migrate by the movement of disconnections of Burgers vector $b$ and step height $h$. Both solutions, with same shear-coupling factor $b = b/h$, correspond to those illustrated in Fig. 4a–d. The grey areas correspond to the groups of atoms moving cooperatively during the process. The alternative Burgers vectors $b_{(\text{Cahn})}$ would correspond to the Cahn mechanism.
impose the shear displacement along this direction (Fig. 8b). The constrained coincidence plane going through A, B, C is thus the new constrained invariant plane. The shear transformation can now be treated as in Section 3.2 above, by the glide of disconnections, with Burgers vector $\mathbf{b}^{\text{(constr)}}$ parallel to the constrained coincidence plane, and with step height $h$. Note that this situation does not correspond to any conventional OR, because the lattices are distorted, and because the coincidence is restricted to the line ABC, as a result, the Burgers vector $\mathbf{b}^{\text{(constr)}}$ does not correspond to any DSC lattice translation. Then, the misfit stresses generated artificially during the procedure are relaxed by introducing a sufficient density of disconnections, in such a way that the average habit plane is tilted back to the original invariant plane (Fig. 8c). The interface can now be described in terms of terraces, parallel to the previous constrained coincidence plane, separated by disconnections with vector $\mathbf{b}$ parallel to the average habit plane (one disconnection at each step). Under such conditions, the boundary motion is achieved by the cooperative motion of all disconnections in their respective terrace planes (Fig. 8c). As discussed by Pond et al. [22], the motion of the disconnections is analogous to a glide process, although their Burgers vector $\mathbf{b}$ is parallel to the invariant plane, not to the terrace plane. The elementary motion of each disconnection, e.g. from C'C'' to B'B'' in Fig. 8c, involves the cooperative displacement and shuffling of the 20 atoms enclosed in each parallelogram (grey area). Note that each of these displacements is smaller than the nearest-neighbor distance, as assumed in the beginning of this work (Section 1).

The general case can thus be treated as the case of coincidence ORs, except that (i) disconnections have Burgers vectors not belonging to any DSC lattice (which
corresponds to the fact that there is no coincidence OR), and (ii) the density of disconnections, which is imposed by the geometry of the interface, is much higher than in the case of a coincidence OR.

3.4. Summary

The different modes of conservative motion of tilt GBs can thus be classified as follows, from the most general case to the most particular one:

- Non-symmetrical boundaries parallel to irrational planes, associated with non-coincidence OR, which can migrate by the glide motion of a high density of interface dislocations on terraces. These disconnections have well-defined Burgers vectors, although not of the DSC type.
- Grain-boundaries, in low-index planes parallel to a dense direction of the DSC lattice, associated with coincidence ORs. These boundaries are most often symmetrical, and they can migrate by the glide motion of DSC dislocations in the interface.
– Grain-boundaries as above (low-index planes parallel to a dense direction of the DSC lattice, associated with coincidence ORs), where the Burgers vector of the DSC lattice is such that the undistorted direction rocking during the rotation is of <100> or <110> type. These boundaries are symmetrical, and their migration can also be described by the Cahn model.

– Grain boundaries with coincidence ORs, migrating by pure atomic shuffling inside each cell of the CSL. There is no shear associated with the migration, the boundary plane can be in any habit plane, and the migration requires no dislocation motion in the interface.

The range of new possibilities of migration-induced shear, given by the general model, is illustrated in Table 1. The values of the coupling factor, $\beta$, and those of the corresponding rotation angles, $\varphi_1$ and $\varphi_2$, have been computed for all couples of motifs defined in Fig. 2. When several couples yield the same result, the redundant results in italic must be disregarded. Then, among the 28 (14 × 2) remaining significant solutions, two ones are trivial because they yield $\varphi = 0$. Among the 26 remaining ones, four ones correspond to the DSC model (in bold), and a single one corresponds to the situation treated by Cahn (the top-left, for $\varphi_1 = 159.95^\circ$). This shows that the general model offers a much larger range of possibilities than the DSC and Cahn models.

4. General tendencies of random boundaries in a polycrystal subjected to a uniaxial deformation

The above description shows that many shear–migration coupling processes can exist, corresponding to various rotations, interface planes, shear directions and coupling factors. The underlying physical mechanism is, however, probably limited to rather small motifs containing sufficiently few atoms to be able to move cooperatively. Table 2 shows several possible low-index rotation axes and corresponding vectors $u$ and $v$. It is clear that high-index rotation axes, and high-index directions of $u$ and $v$, yield increasingly less dense motifs, in which shuffling becomes increasingly difficult.

In three dimensions, it is inferred that boundary dislocations do not move as a whole, by the shuffling and shear of all atoms along their line. They rather move by series of small-scale shear and shuffling of motifs in adjacent planes, by a mechanism similar to the propagation of a kink.

In the case of pure tilt boundaries (i.e. edge-on GBs in Figs. 6–8), grain boundary dislocations can be pure edge (i.e. parallel to the edge-on rotation axis in Figs. 6–8), pure screw (i.e. parallel to the figure plane), or mixed. In all cases, their motion proceeds by the propagation of kinks, corresponding to series of rotation and shear in the intersected motifs.

Table 2
Possible directions of low-index rotation axes, and corresponding $u$ and $v$.

<table>
<thead>
<tr>
<th>Rotation axis</th>
<th>$u$ multiple of $v$</th>
<th>$v$ multiple of $u$</th>
</tr>
</thead>
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<tr>
<td>$&lt;001&gt;$</td>
<td>$1/2&lt;110&gt;$</td>
<td>$1/2&lt;110&gt;$</td>
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<tr>
<td></td>
<td>$&lt;100&gt;$</td>
<td>$&lt;100&gt;$</td>
</tr>
<tr>
<td></td>
<td>$1/2&lt;310&gt;$</td>
<td>$1/2&lt;310&gt;$</td>
</tr>
<tr>
<td></td>
<td>$&lt;100&gt;$</td>
<td>$1/2&lt;110&gt;$</td>
</tr>
<tr>
<td></td>
<td>$1/2&lt;211&gt;$</td>
<td>$&lt;111&gt;$</td>
</tr>
<tr>
<td></td>
<td>$&lt;310&gt;$</td>
<td>$&lt;101&gt;$</td>
</tr>
<tr>
<td></td>
<td>$&lt;210&gt;$</td>
<td>$&lt;210&gt;$</td>
</tr>
<tr>
<td></td>
<td>$&lt;112&gt;$</td>
<td>$&lt;111&gt;$</td>
</tr>
<tr>
<td>$&lt;112&gt;$</td>
<td>$1/2&lt;110&gt;$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$1/2&lt;110&gt;$</td>
<td></td>
</tr>
</tbody>
</table>

Table 1
Values of coupling factor $\beta$, and corresponding rotation angles $\varphi_1$ and $\varphi_2$, calculated in the case of the parallelograms defined in Fig. 2. Results in italic correspond to redundant values, those in bold to the four values given by the DSC model. A single value corresponds to the situation treated by Cahn (top-left, $\varphi_1 = 159.95^\circ$).

<table>
<thead>
<tr>
<th>$\varphi_1$, $\varphi_2$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varphi_1 = 159.95^\circ$ (233)</td>
<td>$2 \sqrt{2} \times 4$</td>
</tr>
<tr>
<td>$\varphi_1 = 0$</td>
<td>$\beta = 0.353$</td>
</tr>
<tr>
<td>$\varphi_2 = 20.05$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 19.00$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 43.44$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 24.24$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 57.35$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 12.09$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 33.89$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 102.31$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 51.83$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 20.56$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 60.47$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_1 = 109.47(23)$</td>
<td>$\beta = 0.433$</td>
</tr>
<tr>
<td>$\varphi_2 = 50.48(211)$</td>
<td>$\beta = 0.433$</td>
</tr>
</tbody>
</table>


As shown in part I [1], the same migration-induced shear mechanism can be transposed to all mixed boundaries deduced from the pure tilt ones considered above, by rotation around the shear direction. However, increasing the twist component always decreases the shear coupling factor, \( b \), in such a way that boundaries with large tilt components (\( h \) almost parallel to the boundary plane) are expected to be the most mobile ones under stress.

Fig. 9 shows that during uniaxial deformation, the resolved shear stress on a pure tilt boundary is proportional to the Schmid factor \( SF = \cos(T \cdot N) \cos(T \cdot b) \), where \( T \) is the direction of the load axis, and \( N \) is the normal to the boundary plane. As for dislocation glide, the highest Schmid factor and highest resolved stress are thus obtained for \((T, N) = (T, b) = 45^\circ\). Under such conditions, the most favored rotation axis \( \theta \) should be perpendicular to the load axis.

The three above conditions—(i) \( \theta \) parallel to a dense direction, (ii) \( \theta \) almost parallel to the boundary plane and (iii) \( \theta \) almost perpendicular to the load axis—are, however, not very restrictive. As a matter of fact, and as shown in part I, there are a fairly large number of rotation axes (and corresponding rotation angles) which can account for a given misorientation. This number is 24 in the general case.

5. Conclusions

The geometrical model presented in this paper allows one to describe the shear–migration coupling of many ordinary GBs, with non-coincidence ORs and irrational habit planes. The main properties of this model can be summarized as follows:

- It generates a large number of solutions, with rotation axes close to dense directions, various rotation angles and interface planes, and coupling factors ranging between a few percent and a few tens of percent.
- In the general case, it involves the glide motion of a high density of disconnections, with Burgers vectors not belonging to any DSC lattice.
- The motion of the disconnections requires the cooperative shear and shuffling of small groups of atoms, within a nearest-neighbor atomic range.
- The DSC and Cahn theories are particular cases of our general model, where both lattices are in a coincidence OR, and where the density of gliding disconnections can be lower.
- This global model allows one to account for a variety of experimental results, including those reported in the part I of this study [1] and concerning fine-grained Al polycrystals. Because it addresses most GBs and allows strain incompatibilities to be solved by atomic shuffling, this model could help describing the GB-based plasticity observed in nanocrystals.

References

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