SMIG model: A new geometrical model to quantify grain boundary-based plasticity

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Abstract

Stress-assisted grain boundary migration is a mechanism that has proven active in polycrystals but that relies on a limited number of models. Those models do not apply to general grain boundaries and often fail to reproduce the intensity of the coupling between the migration distance and the produced shear strain. Recently a new geometrical model, entitled the shear migration geometrical (SMIG) model, that is valid for all tilt boundaries has been introduced to account for the low coupling factors observed experimentally. In the present work we propose, on the basis of this model, (i) to determine, for a given tilt grain boundary, the number of possible coupling modes and (ii) to evaluate the shuffling needed to rearrange atoms as the grain boundary migrates. We will show that, for a given grain boundary defined by a misorientation angle and a grain boundary plane, it is almost always possible to find a coupling mode implying the shuffling of up to 20 atoms, supposedly without long-range diffusion. This characteristic is of prime importance in polycrystals where collective grain boundary motions are required to accommodate strain.

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1. General considerations

The strongly enhanced mechanical behavior of nano- and small-grained materials has triggered deep interest in the materials science community. Many research groups are currently trying to identify and quantify alternative plasticity mechanisms that could explain these enhanced properties. Among them, stress-assisted grain growth and grain boundary-based plasticity have received particular attention. Recent experiments based on nanoindentation and in situ straining experiments have proven that grain coarsening occurs under an applied stress [1–5]. Although this effect has been demonstrated in a large range of temperatures both in nanocrystalline and fine-grained metals, its efficiency in strain accommodation is still widely unknown in this class of materials.

To date, work in the domain of polycrystals has been very limited. Because all grain boundaries (GBs) are inter-dependent in a polycrystal, their migration requires a cooperative process. Even though long-range diffusion should assist GB migration in order to reduce strain incompatibilities, it is supposed that a suitable combination of shear–migration coupling modes is preferred.

The ability of a migrating GB to produce a shear strain is related to the coupling factor \( \beta \), which is defined as the ratio of the GB migration distance to the shear displacement parallel to the GB plane. Extensive measurements of this coupling factor, along with the mobility of the corresponding GB, have been performed in bicrystals at intermediate temperature and exclusively in the elastic regime (below the yield stress) [6–8].

Existing coupling models, namely Cahn’s model [9,10] and the displacement shift compete (DSC) dislocation model [11], have received support from experiments in well-defined bicrystals [6,8,12] and simulations [9,13,14], where the expected values of \( \beta \) were reported. During recent
in situ transmission electron microscopy straining experiments, the strain associated with GB migration was measured in a small-grained Al polycrystal by means of the precise monitoring of the GB position and the use of fixed markers inside the grains [1,15]. These experiments, however, returned low values of the coupling factor, which is equivalent to saying that the GB migration produced unexpectedly small amounts of shear strain when compared to the Cahn and DSC models [10,11]. In addition, these models are restricted to coincident GBs, which limit their implementation to general GBs, as found in real polycrystals. A more general model, which is called the shear migration geometrical (SMIG) model, has recently been proposed in order to account for small measured coupling factors [16]. In the present work, we show that the SMIG model can generate a very large number of coupling factors and can account for GB-based plasticity in real polycrystals.

We propose here to determine, on the basis of the SMIG model, the coupling modes as a function of four parameters: the coupling factor, the size of the parallelograms, the misorientation angle and the GB plane.

2. Basis of the SMIG model

This purely geometrical model consists of finding pairs of shear and rotation values able to easily transform one lattice into another. This approach is illustrated first for a \( \Sigma 5 \langle 0 0 1 \rangle 36.87^\circ \) coincident tilt GB (Fig. 1) and then for a general GB (Fig. 2).

In the (0 0 1) square lattice perpendicular to the GB rotation axis, two parallelograms, labelled 1 and 2, embedding four lattice sites are defined in the two adjacent lattices (Fig. 1a). They are chosen in such a way that they can be transformed from one to the other by a simple shear parallel to the GB plane (Fig. 1b). Under such conditions, the SMIG model intends to find the coupling modes for an arbitrary given set of two parallelograms chosen in a common reference lattice by determining both the misorientation angle and the shear.

![Fig. 1. The SMIG model for a coincident GB (here a \( \Sigma 5 \langle 1 0 0 \rangle 36.87^\circ \)). In a given lattice perpendicular to the GB plane, two parallelograms (1 and 2) enclosing the same number of atoms are defined in the two adjacent lattices (a) in such a way that they can be transformed from one to another by a simple shear parallel to the GB plane (b). The coupling factor is then \( \eta/m \). The two parallelograms can be defined in the reference lattice of the first parallelogram (open circles) by rotating the second parallelogram by the misorientation angle \( \theta \) along an axis perpendicular to the lattice plane. A shear migration coupling mode is obtained by considering the transformation (rotation and shear) that brings two parallelograms, 1 and 2, into coincidence. This process is equivalent to the repeated dislocation glide between equivalent positions along the GB plane leading to the motion of the step parallel to the GB and a migration perpendicular to the GB. This glide is accompanied by atomic shuffling inside the grey area, which is the size of the parallelograms (c).](image-url)
transformation. The GB plane is then defined by the shear direction and the rotation axis.

For coincident misorientations, DSC dislocations with a Burgers vector \( \mathbf{b}_{\text{DSC}} \) gliding in the interface plane between positions A and B are able to propagate the shear and the migration over the distance \( h \) between (1) and (2) (Fig. 1b).

Indeed, these dislocations, associated with steps called disconnections, can move repeatedly between equivalent positions, namely the initial position (i) and the final position (f). This glide induces then the motion of the step from (i) to (f) (Fig. 1c). The corresponding coupling factor is \( \frac{\mathbf{b}_{\text{DSC}}}{h} \).

Fig. 2 illustrates the SMIG model for a non-coincident \( h_{100} \) pure tilt GB. In the two \( 001 \) adjacent lattices, the two parallelograms labelled 1 and 2 (Fig. 2a) are chosen in such a way that they can be transformed from one to the other by a simple shear (Fig. 2b). However, contrary to the coincident case, this configuration imposes the condition that the GB plane is not a rational plane of the two lattices. Thus no DSC dislocation can be defined, since there is no displacement vector that repeats periodically along the GB plane. However, a dislocation associated with a step can be defined as in the case of a coincident GB, its Burgers vector \( \mathbf{b} \) being defined as the difference between the shear at the bottom and the top of the step, i.e. \( \mathbf{b} = \mathbf{s}_1 - \mathbf{s}_2 \) (Fig. 2c). Note that \( \mathbf{b} \) has irrational coordinates in both lattices. The corresponding coupling factor is \( \frac{\mathbf{b}}{h} \).

In order to obtain the expected average GB plane, several terraces and steps are required. The repeated glide of dislocation along terraces between positions leads to the motion of the step parallel to the terrace and then to a migration of the GB. (d) Smaller parallelograms lead to the same coupling mode using a Burgers vector and a step height that are half the size.

Fig. 2. The SMIG model for a general GB (here a GB \( 100 \rightarrow 25.43^\circ \)). The same description (a and b) as in Fig. 1 can be made except that in this configuration the GB plane is irrational. This determines that no coincident lattice can be defined. Migration operates via the glide of dislocations associated to a step of height \( h \) along terraces and atomic shuffling in the grey area (c). The Burgers vector of the dislocation can be defined as the difference between the shear produced at the top and the bottom of the step, i.e. \( \mathbf{b} = \mathbf{s}_1 - \mathbf{s}_2 \). In order to follow the average GB plane, several terraces and steps are required. The repeated glide of dislocation along terraces between positions leads to the motion of the step parallel to the terrace and then to a migration of the GB. (d) Smaller parallelograms lead to the same coupling mode using a Burgers vector and a step height that are half the size.

3. Results

In the first part of this section, we propose a methodology to compute the different solutions. In the second part, we show the relations between the misorientation angle (\( \theta \)), atoms at parallelogram corners to move by a simple shear due to the glide of a disconnection from (i) to (f). Meanwhile, atoms inside the grey area need to shuffle between encircled positions. Three atoms have to shuffle in Fig. 1c and two in Fig. 2c along directions different from the shear direction. This result can be generalized to find that \( N - 1 \) atoms are expected to shuffle when considering parallelograms of size \( N \). The necessity of atomic shuffling in shear migration coupling has been pointed out by Bilby and Crocker in their theory of twinning [18].

It should be noted that several parallelograms can yield the same final result. For instance, in Fig. 2d, the choice of the step height, which depends on the amplitude of the Burgers vector, is not minimum. Indeed, choosing a Burgers vector of half the size, \( \mathbf{b}/2 \), leads to a step with half the height, \( h/2 \), and a lower number of shuffled atoms (one in this case). This happens because a second couple of parallelograms of half the size, i.e. embedding two atoms, leads to the same coupling factor as shown in Fig. 2d. This shows that coupling modes can often be obtained through different ways, depending on the choice of the Burgers vector. However, because the shuffling distances are very small and do not depend on the parallelogram size, the number of shuffling atoms should be minimum. It is thus reasonable to think that a given coupling mode will operate using the smallest possible parallelogram size.
the GB plane \((V)\), the size of parallelograms \((N)\) and the coupling factor \((\beta)\). We finally discuss the results.

3.1. Methodology

As already shown in Figs. 1 and 2, the SMIG model consists of (i) defining parallelograms in a quadratic lattice by shearing an original rectangle drawn along the two orthogonal \(Ox\) and \(Oy\) directions and (ii) relating them by a rotation and a shear transformation. These two procedures are detailed below.

(i) The parallelograms are defined by using an original rectangle from which couples of parallelograms are derived. Let \(\{a, b\}\) be the starting rectangle with side \(\bar{a} = k\bar{u}\) and \(\bar{b} = k'\bar{v}\) (\(\bar{u}\) and \(\bar{v}\) being the unit lattice vector along \(Ox\) and \(Oy\) respectively, and \(k, k'\) being integers). Let \(S(x, p/b)\) and \(S(y, q/a)\) be the shear transformations along \(Ox\) and \(Oy\) with amplitudes \(plb\) and \(qla\), respectively, where \(a = k||\bar{u}||, b = k'||\bar{v}||, p = i||\bar{u}||, q = j||\bar{v}||, i\) and \(j\) being integers. Combinations of these elementary shears lead to a large number of parallelograms. For the sake of simplicity, we restrict the following to a comparison of couples of parallelograms that can be transformed into each other by a combination of two shears, as described by the transformation

\[
S(x, p/b; y, q/a) = S(y, q/a) \circ S(x, p/b)
\]

though a similar methodology, not shown below, can be carried out using the shear transformation

\[
S(y, q/a; x, p/b) = S(x, p/b) \circ S(y, q/a)
\]

The fact that parallelograms should scale with the lattice periodicity imposes restrictions on the \(p\) and \(q\) values, as explained in Appendix A1. In Fig. 2, for instance, we have \((N, p_1, q_1, p_2, q_2) = (4, 1, 0, 1)\).

(ii) It is now sufficient to determine how couples of motives can be transformed into each other by a combination of shear and rotation. The shear is characterized by the shear factor \(\beta\), which depends on \(plb\) and \(qla\), and by the shear direction or the invariant direction. For a couple of parallelograms, two possible rotation angles can be found that bring two common invariant directions of the shear parallel to each other. Thus, for a couple of parallelograms both the two angles and the two directions are needed.

Fig. 3 shows how we proceed. From the original rectangle \(\{a, b\}\), with sides parallel to \(\bar{u}\) and \(\bar{v}\), we can define a couple of parallelograms, denoted 1 and 2, by applying two shear transformations, \(S(x, p_1/b; y, q_1/a)\) and \(S(x, p_2/b; y, q_2/a)\), respectively. The SMIG model consists of finding the rotation \(r(\theta)\) of angle \(\theta\) around the rotation axis perpendicular to the GB plane \((V)\), the size of parallelograms \((N)\) and the coupling factor \((\beta)\). We finally discuss the results.

Fig. 3. Description of the method used to compute the different coupling modes for quadratic lattices. Starting from an initial rectangle \(\{a, b\}\), a couple of parallelograms are defined using shear transformations, denoted \(S(p/b, q/a)\). The two parallelograms can be transformed from one to the other using an appropriate shear and rotation. Under the plane transformation \(r(\theta) \circ S(x, p_1/b; y, q_1/a) \circ S^{-1}(x, p_1/b; y, q_1/a)\), two invariant directions, \(V1\) and \(V2\), can be defined. The coupling factor \((s/m)\) is simply derived from the angle between the two invariant directions.
to \( \vec{a} \) and \( \vec{b} \), which allows parallelograms 1 and 2 to be related by a simple shear. In order to find the rotation angle \( \theta \), we search for the invariant directions of the shear transformation that bring parallelograms 1 and 2 into coincidence. These directions can be defined in the two parallelograms in such a way that, by applying (1) \( S^{-1}(x, p_1/b; y, q_1/a) \), (2) \( S(x, p_2/b; y, q_2/a) \) and (3) \( r(\theta) \) sequentially, the invariant direction defined in the first parallelogram becomes parallel to the invariant direction defined in the second one. In other words, we search for vectors \( \vec{V} = \begin{pmatrix} X \\ Y \end{pmatrix} \) that are unchanged under the transformation

\[
\begin{align*}
\begin{pmatrix} X \\ Y \end{pmatrix} &= r(\theta) \circ S(x, p_2/b; y, q_2/a) \circ S^{-1}(x, p_1/b; y, q_1/a).
\end{align*}
\]

The coupling factor \( \beta \) can then be deduced from the angle between the two invariant directions \( x = (V_1, V_2) \) by the following equation (cf. Fig. 3):

\[
\beta = \pm \tan \left( \frac{\pi}{2} - \alpha \right)
\]

Note that in this model the coupling factor can be either positive or negative, depending on the sign of the disconnection’s Burgers vector.

The whole procedure (i) and (ii) can be carried out using the matrix formalism of planar transformations as detailed in the Appendices A1 and A2.

In the general case, where the lattice is not quadratic, one must start with a parallelogram defined along two dense directions, \( \vec{a} \) and \( \vec{b} \), of the lattice. Applying the SMIG model then consists of shearing this original parallelogram in directions parallel to \( \vec{a} \) and \( \vec{b} \). This can be done using a change in the lattice basis as described in Appendix A2.

Vectors \( V_1 \) and \( V_2 \) and the quantities \( \theta_1, \theta_2 \) and \( \beta \) have been computed using Scilab software\(^1\) for \( (001), (110), (111) \) and \( (2\ 1\ 0) \) lattice planes, using integers ranging between \(-2\) and \(2\) for values of \( p_1, p_2, q_1 \) and \( q_2 \) and \( k \), \( k' \), being integers ranging between \(1\) and \(20\). In the following, a coupling mode will be described by \((N, p_1, q_1, p_2, q_2)\), with \( N = kk' \) corresponding to the number of lattice sites enclosed in the parallelogram.

3.2. Complete sets of results

Fig. 4a shows a plot of \( \beta \) as a function of the misorientation angle \( \theta \) for a \([1\ 0\ 0]\) tilt GB, obtained for parallelograms embedding only one lattice site (no shuffling). We restrict ourselves here to values of \(0 \leq \beta \leq 5\). A similar plot is obtained for parallelograms embedding two lattice sites in Fig. 4b (one shuffling per elementary step motion).

This shows that:

- For a given misorientation angle, several coupling modes can be obtained. For instance a \( \Sigma 5\ (1\ 0\ 0) \)

\[
368.7^\circ \text{ yields two coupling factors for } N = 1, \text{ namely } 1 \text{ and } 4 \text{ (Fig. 4a, but see also Fig. 1).}
\]

- Coupling modes obtained for \( N = 1 \) (Fig. 4a) are also obtained for \( N = 2 \) (Fig. 4b). This arises because identical coupling modes can be obtained using a Burgers vector and a parallelogram that are both twice as large.

- A given coupling factor can be obtained with several misorientation angles. This arises for two reasons: first, because, according to Eq. (2), two misorientation angles yield the same coupling factor, e.g. \( \theta = 14^\circ \) and \( \theta = 137^\circ \) yield \( \beta = 3.6 \), and second, because of the lattice symmetry, as explained below.

- The number of possible coupling factors increases and the lowest coupling factor value decreases as the number of embedded atoms increases.

- The ratio of the number of coupling modes for non-coincident GB (encircled crosses) over the total number of coupling modes increases with the number of embedded atoms.

Fig. 4 clearly exhibits a mirror symmetry along the \( \theta = 45^\circ \) and \( \theta = 90^\circ \) lines. This arises because of the fourfold rotation symmetry of the \((1\ 0\ 0)\) lattice plane, and because the misorientation angles can be taken either positive or negative. Table 1 shows equivalent coupling modes obtained by choosing all possible couples of equivalent parallelograms related by the fourfold rotation \( R(\pi/2) \). Eight equivalent coupling modes can be found for a coupling factor of \( 1 \) with four different misorientation angles \( \pm \theta \) (modulo \( \pi/2 \)) and four GB planes. It can be said that coupling modes for GB with a rotation parallel to the \((1\ 0\ 0)\) direction (in the following denoted \((1\ 0\ 0)\) GB) have a degeneracy of \( 4 \). Note the other coupling mode \( \theta = 48.18^\circ \) on the diagonal of the table. For the same reasons, coupling modes in \((1\ 1\ 1), (1\ 1\ 0)\) and \((2\ 1\ 0)\) GBs have degeneracies of \(3, 2\) and \(2\) respectively.

Fig. 5 shows a plot of the minimum value of the coupling factor \( \beta_{\text{min}} \) as a function of the parallelogram size \( N \) for \((1\ 0\ 0)\) (crosses), \((1\ 1\ 0)\) (dots), \((1\ 1\ 1)\) (triangles) and \((2\ 1\ 0)\) (stars) tilt GBs. The decrease in \( \beta_{\text{min}} \) follows a \( \beta_{\text{min}}/N \) law exactly, with \( \beta_{\text{min}} \) being the minimum coupling factor for \( N = 1 \). The decrease of \( \beta \) with increasing \( N \) is also observed for the DSC dislocation model. As large index GBs with a large CSL unit cell are invoked, both a small DSC dislocation Burgers vector within the CSL lattice and a larger step height can be chosen.

In Fig. 6, each dot represents a possible coupling mode associated to a value of \( N \) and \( \theta \) for a \((1\ 1\ 0)\) tilt GB, restricted to \( N \leq 10 \). It can be seen that the plot is very dense. Similar plots for other GBs are also very dense. This shows that it is almost always possible to find a coupling mode for an arbitrary misorientation angle. However, each solution corresponds to a specific GB plane and a given coupling factor. In order to better represent the different solutions, we need to investigate the relationships between \( \beta, \theta \) and \( V \).

Fig. 7 shows \( \theta - \beta \) (Fig. 7a), \( \theta - \phi \) (Fig. 7b) and \( \phi - \beta \) (Fig. 7c) plots for \((1\ 1\ 0)\) GB, \( \phi \) being the angle between

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\(^1\) Scilab is an open source software governed by the CeCILL licence.
Fig. 4. Coupling factor plot ($f$) as a function of the misorientation angle ($\theta$) obtained using couples of parallelograms of size $N = 1$ (a) or $N = 2$ (b). Low index coincident GBs are located along the dashed lines. Coupling modes for non-coincident GBs are indicated by encircled crosses.
the invariant shear direction (or the GB plane) and the Ox direction, i.e. \( \phi = \arctan(Y/X) \) where \( X \) and \( Y \) are the coordinates of the \( V \) vector. The \( \theta-\beta \) plot (Fig. 7a) shows the expected symmetry for the (1 1 0) lattice plane along the \( \theta = 90^\circ \) line. Several coupling factors are available for \( \Sigma 9 \) and \( \Sigma 3 \) coincident GBs. This is due to the large number of possible Burgers vectors that can be chosen within the CSL unit cell. Out of these particular values of \( \theta \), the plot shows mainly a chain-like structure with closely distributed modes. Note that the structure is especially dense at small angles (modulo 180°). Similar plots exhibiting the chain-like structure can be obtained with other types of GB.

The \( \theta-\phi \) plot (Fig. 7b) and the \( \phi-\beta \) plot (Fig. 7c) show respectively a mirror symmetry along the \( \theta = 90^\circ \) line and central symmetry with respect to the point \( \phi = 0, \theta = 90^\circ \). These properties come from the lattice symmetry, because the two misorientation angles \( \theta \) and \(-\theta \) (modulus 180°) yield the same coupling factor \( \beta \) but opposite values \( \phi \). In both figures, the chain-like structure is also visible.

<table>
<thead>
<tr>
<th>Parallelogram 1</th>
<th>Parallelogram 2</th>
<th>( \theta )</th>
<th>( V )</th>
<th>( \theta )</th>
<th>( V )</th>
</tr>
</thead>
<tbody>
<tr>
<td>{1, 0}</td>
<td>{-1, 0}</td>
<td>( \pm 90 - 36.87^\circ )</td>
<td>( -130 )</td>
<td>( \pm 90 + 36.87^\circ )</td>
<td>( 3-10 )</td>
</tr>
<tr>
<td>{0, 1}</td>
<td>{0, -1}</td>
<td>( 36.87^\circ )</td>
<td>( V ) irrational</td>
<td>( 48.18^\circ )</td>
<td>( 310 )</td>
</tr>
</tbody>
</table>

Fig. 6. Possible coupling modes (dots) for a (1 1 0) tilt GB.
The structure of one chain is complex and results from the superimposition of several families of coupling modes. The structure of the chain denoted A is described in Fig. 9. It is composed of six intricate families, each one composed of a series of coupling modes with identical values of \( q_1, q_2 \) and \( \Delta = p_1 - p_2 \) but different values of \( N \) (in Fig. 9a only the modes with \( N \leq 20 \) are shown).

The lowest part of chain A is shown in Fig. 9b. Only the modes corresponding to \( q_1 = 0 \) and \( q_2 = -1 \) are shown for the sake of simplicity. For these values, it can be shown that the parameters \( \phi, \theta \) and \( \beta \) are given by the following equations:

\[
\phi = \arctan \left( \frac{\sqrt{2N(3\Delta + 2N - \sqrt{3\Delta^2 + 4\Delta N + 4N^2})}}{3\Delta + 4N} \right)
\]

(4)

\[
\theta = 2 \arctan \left( \frac{\sqrt{2(2N - \Delta + \sqrt{3\Delta^2 + 4\Delta N + 4N^2})}}{2(\Delta + 4N)} \right)
\]

(5)

and

\[
\beta = \sqrt{\frac{3\Delta^2 + 4\Delta N}{2N^2}} + 2
\]

(6)

According to these equations, all solutions fall on a single curve. The first family with \( \Delta = -1 \) starts at \( N = 20 \) (maximum chosen value) and continues with decreasing values of \( N \). The second family, with \( \Delta = -2 \), also starts at \( N = 20 \), where the first one has a solution for \( N = 10 \) (this occurs because \( \Delta = -1, N = 10 \) and \( \Delta = -2, N = 20 \) yield the same value of \( \phi \) and \( \theta \)). The third family starts at higher values of \( \phi \) and \( \theta \), etc.

Although the relations between \( \beta, \theta \) and \( \phi \) are complex, Eq. (6) shows that the coupling factor decreases mainly as \( 1/N \), in agreement with Fig. 5. The closeness of the solutions suggests that a continuous chain-like structure is expected at the limit of infinitely large values of \( N, p \) and \( q \).

Other chains obey similar rules, with slightly different parameters.

One particular interesting chain is shown in the grey\(^2\) colour in the three plots of Fig. 8. It is composed of several families of coupling modes verifying \( \Delta = p_1 - p_2 \) ranging from \(-4\) to \(-1\) and \( q_1 = q_2 = -2 \). It can be demonstrated that the corresponding equations are:

\[
\phi = \arctan \left( \frac{2\sqrt{2(N + 2\Delta)}}{4N} \right)
\]

(7)

\[
\theta = 2 \arctan \left( \frac{9\sqrt{2}\Delta}{4N} \right)
\]

(8)

and

\[
\beta = \frac{9\sqrt{2}\Delta}{2N}
\]

(9)

\(^2\) For interpretation of color in Figs. 8, 9 and 10, the reader is referred to the web version of this article.
Combining Eqs. (7) and (8) leads to the well-known formula given by Cahn and Taylor [10]:

\[ \beta = 2 \tan \left( \frac{\theta}{2} \right) \]  

Because \( \tan \left( \frac{\pi}{4} \right) = \frac{m}{n} \) with \( m \) and \( n \) integers, the two adjacent lattices have coincident positions and thus this chain describes only coincident GB. However, except the \( \Sigma 3 \) GB, all other coincident GBs have a high \( \Sigma \) index.
Fig. 9. Details of the chain A shown in Fig. 8. (a) The chain is composed of six different families of coupling modes, each of them having the same values of \( q_1 = 0 \) and \( q_2 = \frac{1}{2} \) or \( -\frac{1}{2} \) and a given value of \( p_1 - p_2 \). (b) Details of the insert shown in (a): each of the intricate families of coupling modes (black, red and blue dots) are composed of coupling modes that have decreasing values of \( N \) (indicated above each dots) with increasing \( \theta \).
and their corresponding coupling modes require a lot of shuffling.

4. Discussion

4.1. Model limitations

The large number of available coupling factors given by the SMIG model has been computed under the conditions specified above. This approach does, however, suffer from two limitations:

- Parallelograms are derived from only two shears of small amplitude (p and q values ranging between −2 and 2).
- Only couples of parallelograms originating from the same basis {a, b} are used. We then miss couples of parallelograms originating from different bases of the same size.

These two limitations are expected to lower the number of real possible coupling modes, but do not change the general result. The results above indicate that, for an arbitrary set of θ, β and V, we are almost always close to an available coupling mode.

4.2. Activation energy

Since θ and V̂ are fixed by the GB geometry, it is expected that the GB will choose to migrate with one of the available closest and easiest coupling modes. This choice depends on (i) the driving stress, (ii) the GB mobility and (iii) the necessity to accommodate a given strain. This latter point is especially important in polycrystals, where GB migrations are not independent. As shown in Ref. [8], the stress-driven GB mobility exhibits a temperature dependence indicating that thermally activated processes control GB migration. As the SMIG model is a purely geometrical model, the question of the GB migration activation enthalpy for a given coupling mode cannot be simply addressed. However, some general ideas can be drawn. As in the DSC dislocation theory, GB migration operates in the SMIG model via the propagation of dislocation-type defects in the interface plane associated with the shuffling of atoms. This process is supposed to be a thermally activated process, because it usually requires collective atomic rearrangements over several saddle positions with abnormal interatomic distances. The GB migration activation enthalpy H_{GBM} for a coupling mode should then depend on different contributions:

- the disconnection nucleation enthalpy H_{nucl},
- the disconnection propagation enthalpy, which decomposes into the shuffling enthalpy H_{shuff} of atoms inside the disconnection step (corresponding to atoms inside parallelograms), and the shear activation enthalpy H_{shear}, which corresponds to the shear displacement of atoms at parallelogram corners.

The shuffling enthalpy is expected to be a growing function of the number of shuffled atoms. The disconnection nucleation enthalpy will depend on the step height and the Burgers vector, and the shear activation enthalpy will depend on the Peierls potential along the terrace.

Since the GB geometry is fixed, the GB can migrate either according to a coupling mode exactly described by the SMIG model with a reasonably low number of shuffled atoms (exact solutions) or according to the closest available SMIG solution (approximated solutions). In the first case, the expected GB migration activation enthalpy is H_{GBM} + H_{shuff} + H_{nucl} + H_{shear}. In the second case, the migration is expected to require additional long-range diffusion. This is the case when, for example, the GB plane is not planar but V is continuously changing. The activation enthalpy should then be H_{GBM} + H_{shuff} + H_{nucl} + H_{shear} + H_{GRD}, with H_{GRD} the GB self-diffusion enthalpy. However, contrary to classical long-range diffusion mechanisms, such as Coble creep, where every single atom has to be displaced by diffusion processes, stress-driven GB migration in the SMIG model requires the displacement of only a few atoms over large distances, most of them being rearranged under shuffling mechanisms. Thus, the GB mobility can be much higher than expected for “pure” long-range diffusion mechanisms, in agreement with experimental results [1].

GB coupling modes have been investigated recently by several atomistic simulations [13,19–22]. They all show that GB migration is a thermally activated process implying atomic shuffling. Mishin et al. have treated GB migration by a Peierls-type mechanism, where the GBs move along a periodic potential [19–23]. According to these simulations, GB migration occurs at low and intermediate temperatures and high velocity by an incremental motion as soon as the flow stress reaches a critical value. They have shown that for a coincident GB, in a large range of temperature, the migration remains coupled to a given mode and that the critical stress decreases with increasing temperature. In their description, GB migration requires small atomic rearrangements in small structural units along the GB plane associated to the motion of dislocations, as proposed in Cahn’s model [9]. The decrease of the critical stress for GB migration with increasing temperature has also been found in simulations where disconnection motion has been observed [13–20].

This concept of atomic shuffling is also supported by the careful study of Zhang and Srolovitz [21]. From numerical simulations on Σ5 tilt GBs in nickel, they reported that three types of atomic hops are required for GB migration. They found that GB migration is a collective phenomenon implying several types of atomic shuffling that occur sequentially, first parallel to the GB plane and then perpendicular. Some of these atomic hops that require or produce excess volume are expected to be the rate limiting process for GB migration. They found that a large excess volume is correlated to a large GB mobility, and suggested that a correlation exists between GB mobility and GB self-diffu-
sivity. Note that no long-range diffusion is needed in these simulations.

Gorkaya et al. [8] recently measured the coupling factor of GB with several misorientations in the range 0–90° for \(<100>\) tilt GBs. They report a good agreement with Cahn’s theory, even though the data points do not strictly follow the expected dependence of the coupling factor on the misorientation angle. Fig. 10 shows, in superimposition, the experimental data points on a \(\beta - \theta\) plot extracted from Ref. [8] and the coupling modes given by the SMIG model. The data points can be seen to fit well the expected curves \(\beta = 2 \tan(\theta/2)\) (in green) and \(\beta = -2 \tan(\pi/4 - \theta/2)\) (in blue), corresponding to the two Cahn’s coupling modes, especially at a low misorientation angle (modulo 90°). However, some discrepancies at higher misorientation angles can be explained within the SMIG model by considering other possible modes.

In the same study, the authors measured that the activation enthalpy of the shear migration coupling for general GBs. They found smaller activation enthalpies close to coincident GBs. In this situation, since both the disconnection step height and the number of shuffled atoms decrease when the CSL unit cell decreases, we expect a decrease in the activation energy. A minimum is found close to the \(\Sigma 5\ 53.13^\circ\) GB for \(\theta = 55.4^\circ\). In this case, the activation enthalpy is expected to be \(H_{\text{GBM}}(\theta = 55.4^\circ) \approx H_{\text{GBM}}(\theta = 55.13^\circ) + H_{\text{GBD}}\). For a \(\Sigma 5\ 53.13^\circ\) GB and for \(\beta = -0.666\), corresponding to the \((3, -2, 1, 0, -1)\) coupling mode, we expect the shuffling of only two atoms. The difference between the GB migration enthalpies can thus be attributed to the difference in the number of atoms shuffled. The shuffling enthalpy of coupling modes can thus be estimated as being a few tenths of an electronvolt.

5. Conclusions

In this paper we have explored the large variety of shear-coupled GB migration modes within the framework of the SMIG model. These modes are characterized by three parameters: the coupling factor \((\beta)\), the misorientation angle of the GB \((\theta)\) and the GB plane \((V)\). From this study it appears that:

- The SMIG model proposes a broad spectrum of discrete solutions for shear-coupled GB migration. These solutions imply the shuffling of several atoms (limited to 20 in this study).
- For a given GB geometry \((\theta, V)\), there is likely to be a coupling mode with one or several values of the coupling factor \(\beta\). GB migration operates according to the easiest and closest available coupling mode, which may imply a limited amount of long-range diffusion.

This indicates that the SMIG model is an adequate way to describe GB-mediated plasticity in polycrystals, where collective GB migrations involving a large variety of coupling modes are needed to accommodate strain. GB mobility should depend on the amount of shuffling required, but the correlation between the number of atoms shuffled and the activation enthalpy needs further investigation.

Appendix A. Description of the SMIG model by transformation matrices

A1. Quadratic lattices

In the framework of 2-D transformation matrices, Eq. (2) can be written:

\[
C(x/p/b; y/q/a) = C(y/q/a) \cdot C(x/p/b)
\]

\[
= \begin{pmatrix}
1 & 0 \\
q/a & 1
\end{pmatrix}
\begin{pmatrix}
1 & q/b \\
0 & 1
\end{pmatrix}
= \begin{pmatrix}
1 & q/b \\
q/a & q/a \cdot b / m + 1
\end{pmatrix}
\]

(A1)
Considering that all the parallellograms should scale with the lattice, this implies that two corners, e.g. \((a, 0)\) and \((0, b)\), should fall on lattice nodes after a shear of amplitude \(p = i||u||\) and \(q = j||v||\) \((i, j\) integers).

Since

\[
C(x, p/b; y, q/a) \binom{a}{0} = \binom{a}{q} 
\]

and

\[
C(x, p/b; y, q/a) \binom{0}{b} = \binom{p}{b + \frac{ma}{a}}
\]

the condition of the first corner \((a, 0)\) is always fulfilled since \((a, q)\) is the lattice point \(k\hat{u} + j\hat{v}\). However, the condition on the second corner \((0, b)\) implies that the \(y\)-coordinate \(b + \frac{ma}{a}\) is a multiple of \(m||v||\), \(m\) being an integer, i.e.: \[
\left( k + \frac{ij}{k} \right) = m \tag{A2}
\]

In terms of matrices, the SMIG model consists of determining the two eigenvectors of the transformation matrix \(R(\theta) \cdot C(x, p_2/b; y, q_2/a) \cdot C^{-1}(x, p_1/b; y, q_1/a)\) associated to the eigenvalue \(\lambda = 1\), i.e.: \[
R(\theta) \cdot C(x, p_2/b; y, q_2/a) \cdot C^{-1}(x, p_1/b; y, q_1/a) \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} \tag{A3}
\]

where the rotation matrix \(R(\theta)\) is:

\[
R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \tag{A4}
\]

The eigenvectors \(\vec{V}\) are directed along two invariant directions, denoted \(I^1\) and \(I^2\) in Fig. 3. Then, \(\vec{V}\) and the rotation axis define the GB plane.

The condition \(\lambda = 1\) leads to the condition on \(\theta:\)

\[
\det \left( R(\theta) \cdot C(x, p_2/b; y, q_2/a) \cdot C^{-1}(x, p_1/b; y, q_1/a) - I \right) = 0 \tag{A5}
\]

This equation yields two solutions, \(\theta_1\) and \(\theta_2\). Eigenvectors \(V_1\) and \(V_2\) are then found using Eq. (A3) and the values of \(\theta_1\) and \(\theta_2\).

**Appendix A2. Non-quadratic lattices**

To respect the lattice symmetry, one cannot use a rectangle as the starting point of the SMIG model for non-quadratic lattices. In the general case, one must start with a parallelogram defined along two dense directions, \(\vec{u}'\) and \(\vec{v}'\), of the lattice. Applying the SMIG model then consists of shearing this original parallelogram in directions parallel to \(\vec{u}'\) and \(\vec{v}'\). For instance, considering the (1 1 1) lattice, the starting parallelogram can be chosen with side \(\vec{u}' = \hat{e}_1\) and \(\vec{v}' = 0.5\hat{e}_1 + \frac{\sqrt{2}}{2}\hat{e}_2\), where \(\hat{e}_1\) and \(\hat{e}_2\) are unit length vectors in the orthonormal \((O_x, O_y)\) basis (see Fig. 11). The two shear operations of the original parallelogram along these directions are then given by:

\[
P^{-1} \cdot C(x, p_2/b; y, q_2/a) \cdot C^{-1}(x, p_1/b; y, q_1/a) \cdot P, \tag{A6}
\]

where \(P\) is the matrix that changes the basis \(\{\hat{e}_1, \hat{e}_2\}\) to \(\{\hat{u}', \hat{v}'\}\), i.e. the matrix that transforms a given \((x', y')\) vector defined in \(\{\hat{u}', \hat{v}'\}\) into a \((x, y)\) vector defined in \(\{\hat{e}_1, \hat{e}_2\}\), namely

\[
\begin{pmatrix} x \\ y \end{pmatrix} = P \begin{pmatrix} x' \\ y' \end{pmatrix} \tag{A7}
\]

Eq. (A5) becomes then:

\[
\det \left( R(\theta) \cdot P^{-1} \cdot C(x, p_2/b; y, q_2/a) \cdot C^{-1}(x, p_1/b; y, q_1/a) \cdot P - I \right) = 0 \tag{A8}
\]

from which eigenvectors and coupling factors can be deduced, as explained in Section A1.

**References**