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On the auxiliary lattices and dislocation reactions at triple junctions

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Coincidence site and displacement shift complete lattices of triple junctions are analysed. Dislocation reactions at triple junctions are considered. It is shown that in $\alpha = 1$ junctions no trapped residual triple-junction dislocation is geometrically necessary for dislocation transmission between adjoining grain boundaries. However, the situation is different for $\alpha \neq 1$ triple junctions, where in some cases the residual dislocation cannot leave the triple junction for a grain boundary without generating a stacking-fault-like defect.

1. Introduction

This is the third paper in the series on the crystallography of triple junctions of coincidence site lattice (CSL) boundaries. The reader is referred to the two previous papers (Gertsman, 2001*a*,*b*,*c*) for a more detailed introduction to the problem. In those papers, the CSL theory of multicrystallite assemblages, in particular triple junctions, was suggested. However, some questions pertaining to the auxiliary lattices defining the triple junction, *viz* the CSL and its derivative, the displacement shift complete (DSC) lattice, have been either put forth as conjectures or not addressed at all. Knowledge of these auxiliary lattices is needed for computer modelling and analysis of experimental data. The current paper explores the properties of the triple-junction CSL and DSC lattice, and applies the results to the analysis of dislocation interactions at the triple junction. The latter is important for consideration of transmission of sliding from boundary to boundary through the triple junction as well as for general understanding of the dislocation balance in the polycrystal. Although the examples given in the paper relate to the cubic crystal system, the consideration is, in general, not lattice specific. Hence, the conclusions are applicable to an arbitrary crystal lattice.

2. Specifics of coincidence site lattice of a triple junction

The triple-junction CSL is the lattice of sites common to three crystal lattices, *i.e.* it is a sublattice of all the three crystal lattices. It is easy to show that the triple-junction CSL is also a sublattice of all the three CSLs formed by the crystal lattice pairs (grain-boundary CSLs), *i.e.* it is the lattice of sites common to all three grain-boundary CSLs.

Consider a triple junction of the three crystals defined by the lattices Λ_1, Λ_2 and Λ_3 (Fig. 1) with bases $(\mathbf{e}_{11}, \mathbf{e}_{12}, \mathbf{e}_{13})$, $(\mathbf{e}_{21}, \mathbf{e}_{22}, \mathbf{e}_{23})$ and $(\mathbf{e}_{31}, \mathbf{e}_{32}, \mathbf{e}_{33})$, respectively. Denote $\Lambda_C^{\mathrm{GB1}} := \mathrm{CSL}(\Lambda_1, \Lambda_2)$, $\Lambda_C^{\mathrm{GB2}} := \mathrm{CSL}(\Lambda_1, \Lambda_3)$, $\Lambda_C^{\mathrm{GB3}} := \mathrm{CSL}(\Lambda_2, \Lambda_3)$ and $\Lambda_C^{\mathrm{TJ}} := \mathrm{CSL}(\Lambda_1, \Lambda_2, \Lambda_3)$.

Grain-boundary CSLs consist of vectors $\mathbf{c}^{\mathrm{GB1}} \in (\Lambda_1, \Lambda_2)$, $\mathbf{c}^{\mathrm{GB2}} \in (\Lambda_1, \Lambda_3)$, $\mathbf{c}^{\mathrm{GB3}} \in (\Lambda_2, \Lambda_3)$, *i.e.*

$$\mathbf{c}^{\mathrm{GB1}} = \sum_{i=1}^{3} l_{1i}\mathbf{e}_{1i} = \sum_{i=1}^{3} l_{2i}\mathbf{e}_{2i}, \quad \mathbf{c}^{\mathrm{GB2}} = \sum_{i=1}^{3} l_{1i}\mathbf{e}_{1i} = \sum_{i=1}^{3} l_{3i}\mathbf{e}_{3i},$$
$$\mathbf{c}^{\mathrm{GB3}} = \sum_{i=1}^{3} l_{2i}\mathbf{e}_{2i} = \sum_{i=1}^{3} l_{3i}\mathbf{e}_{3i}, \tag{1}$$

where all l are integers. Λ_C^{TJ} consists of vectors $\mathbf{c}^{\mathrm{TJ}} \in (\Lambda_1, \Lambda_2, \Lambda_3)$, *i.e.*

$$\mathbf{c}^{\mathrm{TJ}} = \sum_{i=1}^{3} m_{1i}\mathbf{e}_{1i} = \sum_{i=1}^{3} m_{2i}\mathbf{e}_{2i} = \sum_{i=1}^{3} m_{3i}\mathbf{e}_{3i}, \tag{2}$$

where all m are integers.

Thus, the triple-junction CSL is the CSL of the three grain-boundary CSLs. However, it is not immediately clear whether the triple-junction CSL itself belongs to the same class as grain-boundary CSLs. In other words: Is the triple-junction CSL characterized by the multiplicity factor Σ^{TJ} crystallographically equivalent to some grain-boundary CSL with the same magnitude of the reciprocal density of coincident sites, $\Sigma = \Sigma^{\mathrm{TJ}}$? For $\alpha = 1$ junctions,[1] the answer is obvious and trivial since the triple-junction CSL coincides with the CSL of the boundary with the greatest Σ value and $\Sigma^{\mathrm{TJ}} = \Sigma^{\mathrm{GB}}_{\max}$. Such triple-junction CSLs belong to the class of grain-boundary CSLs characteristic of the given crystal system – they form a subclass characterized by non-prime Σ values.

The answer is not so clear, however, for $\alpha \neq 1$ triple junctions. To show that triple-junction CSLs that cannot be reduced to a grain-boundary CSL do exist, it is sufficient to demonstrate a numerical example. Consider *e.g.* a $\Sigma9$–$\Sigma9$–$\Sigma9$ junction ($\Sigma^{\mathrm{TJ}} = 27$). Fig. 2(*a*) presents a graphic illustration of the $\Sigma^{\mathrm{TJ}} = 27$ triple-junction CSL. The schematic shows the superposition of three simple cubic lattices mutually rotated by 120° about [511], *i.e.* each pair of lattices has the $\Sigma9$ misorientation [this example is considered in detail in

[1] α is the parameter in the Σ combination rule: $\Sigma_3 = \Sigma_1\Sigma_2/\alpha$ (Gertsman, 2001*a*).

Gertsman (2001*a*)]. Two grain-boundary CSLs with $\Sigma = 27$ exist, see *e.g.* Grimmer *et al.* (1974). Obviously, the $\Sigma^{\rm TJ} = 27$ CSL cannot be the same as the $\Sigma27a$ grain-boundary CSL because, while the former is characterized by the coincidence of every third crystal lattice site in every ninth (511) plane, all lattice sites are in coincident positions in every 27th (511) plane in the latter (this simply follows from the fact that 180°[511] is one of the descriptions of the $\Sigma27a$ misorientation). The $\Sigma27b$ configuration is displayed in Fig. 2(*b*). The two lattices in Fig. 2(*b*) are shown having the 60°[511] misorientation, which is one of the equivalent descriptions of the $\Sigma27b$ misorientation. At first glance, it looks as if the $\Sigma27b$ grain-boundary CSL is the same as the $\Sigma^{\rm TJ} = 27$ CSL: the coincidence occurs for every third crystal lattice site in every ninth (511) plane. However, the CSL planes parallel to (511) have different shifts for the two CSLs (see Fig. 2). Therefore, the two CSLs are different. Formally, this can be shown as follows.

The unit cell of the $\Sigma27b$ CSL can be described by the following basis:

$$C_{\Sigma27b} = \begin{pmatrix} -1 & -1 & 2 \\ 4 & 1 & 0 \\ 1 & 4 & -1 \end{pmatrix}. \qquad (3)$$

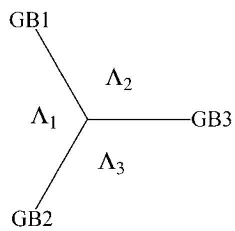

Figure 1
Schematics of a triple junction.

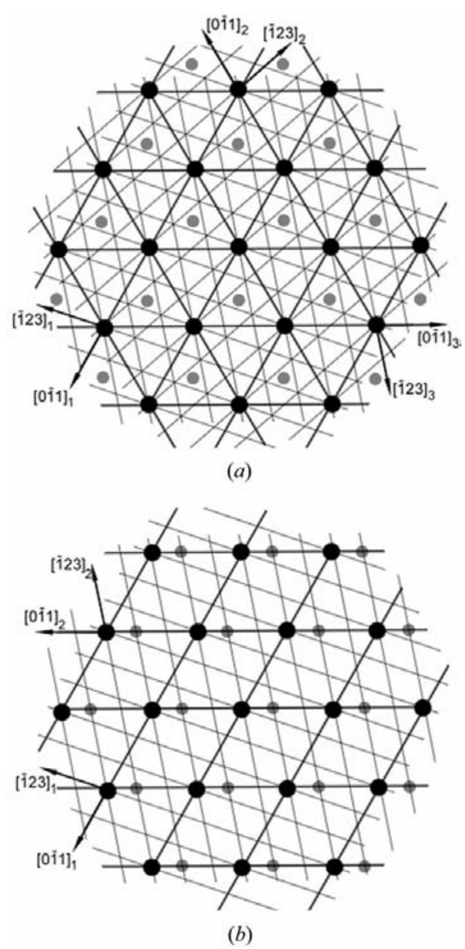

Figure 2
(*a*) Triple-junction CSL with $\Sigma^{\rm TJ} = 27$. (*b*) Grain-boundary CSL $\Sigma27b$. (511) projection. Coincident sites in the plane of the figure are shown by the black circles, smaller grey circles denote coincident sites in the plane $3^{1/2}a$ below the plane of the figure.

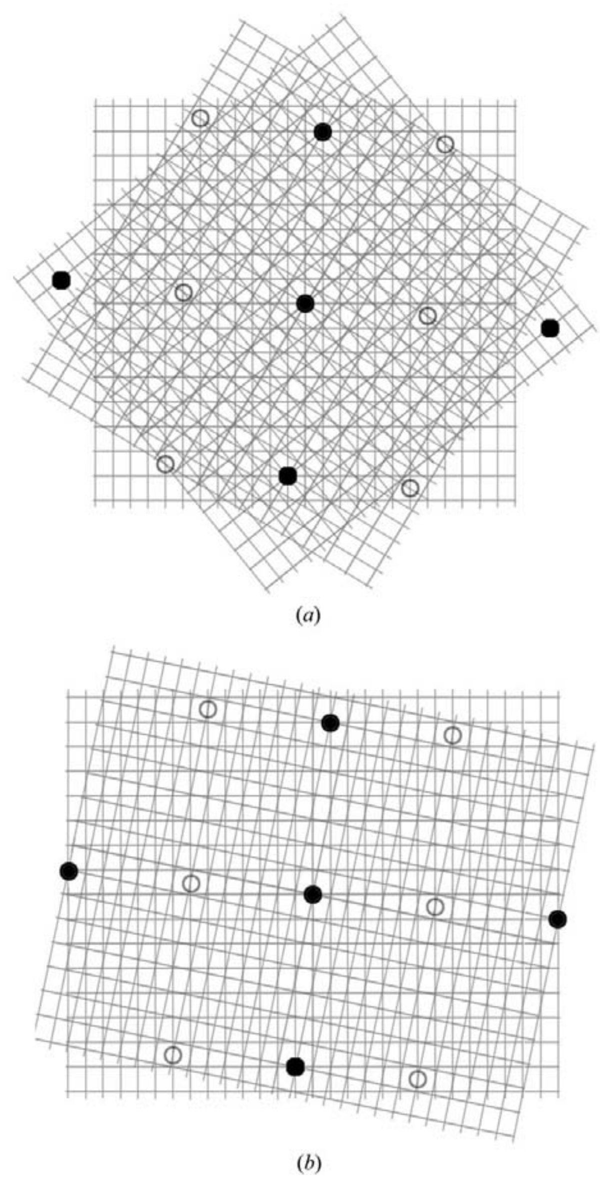

Figure 3
Comparison between CSLs (*a*) $\Sigma^{\rm TJ}99$ and (*b*) $\Sigma99a$. (110) projection. Black circles denote coincident sites in the plane of the figure, open circles denote coincident sites at height $2^{-1/2}a$.

This unit cell can be reshaped to the form given in Table 1 of Grimmer *et al.* (1974), but we have chosen the first two basis vectors in the (511) plane for an easier comparison with Fig. 1.

The basis of the $\Sigma^{\rm TJ}=27$ CSL can be described by

$$C_{\Sigma^{\rm TJ}27}=\begin{pmatrix}-1&-1&2\\4&1&1\\1&4&-2\end{pmatrix}. \qquad (4)$$

One can easily check that the unit-cell volumes, calculated *e.g.* as $\mathbf{e}_1\cdot(\mathbf{e}_2\times\mathbf{e}_3)$, are equal to 27 in both cases (assuming the crystal lattice constant $a=1$), *i.e.* these are indeed $\Sigma=27$ CSLs. The two CSLs differ in the third basis vector. Vector $\mathbf{e}_3$ of the $\Sigma27b$ CSL does not belong to the lattice described by the unit cell $C_{\Sigma^{\rm TJ}27}$, *i.e.* it cannot be obtained by a linear combination of the basis vectors of the $\Sigma^{\rm TJ}=27$ CSL. Similarly, vector $\mathbf{e}_3$ of the $\Sigma^{\rm TJ}=27$ CSL does not belong to the lattice described by the unit cell $C_{\Sigma27b}$.

Yet, the conclusion that all $\alpha\neq1$ triple-junction CSLs differ from grain-boundary CSLs is not correct. A counterexample is presented in Fig. 3. Fig. 3(*a*) displays the superposition of three crystal lattices having the $\Sigma9$, $\Sigma33a$ and $\Sigma33c$ grain-boundary misorientations. This example of an $\alpha\neq1$ triple junction was also considered in Gertsman (2001*a*), it is characterized by $\Sigma^{\rm TJ}=99$. Fig. 3(*b*) shows two lattices misoriented by 11.54° about [110] and forming the $\Sigma99a$ grain-boundary CSL. It is evident that the two CSLs are the same, which can also be shown in a different way.

The orientations of the three crystallites in the $\Sigma9$–$\Sigma33a$–$\Sigma33c$ triple junction can be represented as

$$A=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad B=\frac{1}{9}\begin{pmatrix}8&1&-4\\1&8&4\\4&-4&7\end{pmatrix},$$
$$C=\frac{1}{33}\begin{pmatrix}25&8&-20\\8&25&20\\20&-20&17\end{pmatrix}. \qquad (5)$$

Let us add the fourth crystallite with the orientation

$$D=\frac{1}{99}\begin{pmatrix}98&1&14\\1&98&-14\\-14&14&97\end{pmatrix}. \qquad (6)$$

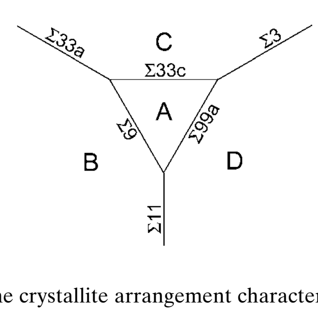

Figure 4
Schematics of the crystallite arrangement characterized by the same CSL $\Sigma=99$.

The four crystal orientations can form six grain boundaries with the following misorientations: A/B–$\Sigma9$, A/C–$\Sigma33c$, A/D–$\Sigma99a$, B/C–$\Sigma33a$, B/D–$\Sigma11$ and C/D–$\Sigma3$. Four triple junctions are possible among the four given crystals, *viz* A–B–C, A–B–D, A–C–D and B–C–D. Interestingly, three of them are characterized by $\Sigma^{\rm TJ}=99$: two $\alpha=1$ junctions, $\Sigma9$–$\Sigma11$–$\Sigma99a$ and $\Sigma3$–$\Sigma33c$–$\Sigma99a$, and an $\alpha\neq1$ junction $\Sigma9$–$\Sigma33a$–$\Sigma33c$ (schematics containing all these triple junctions are shown in Fig. 4). It is immediately clear that the first two junctions have the triple-junction CSLs the same as grain-boundary CSL $\Sigma99a$. Moreover, any configuration of the four crystallites will be characterized by the multi-CSL with $\Sigma^{\rm tetra}=99$, which is again the same as $\Sigma99a$ [see Gertsman (2001*c*) for different spatial arrangements of grains in the tetracrystal and for the details of calculating Σ]. Then, all the triple-junction CSLs in the arrangement shown in Fig. 4 must completely coincide with each other and with the tetra-CSL. Hence, the CSL of the A–B–C ($\Sigma9$–$\Sigma33a$–$\Sigma33c$) junction characterized by $\Sigma^{\rm TJ}=99$ cannot be different from $\Sigma99a$ since otherwise the superposition of the grain-boundary and triple-junction CSLs in Fig. 4 would produce a tetra-CSL with $\Sigma>99$.

The above example shows that the same triple-junction CSL can characterize different triple junctions. The following remote analogy could be suggested for this property – a grain-boundary CSL describes different spatial arrangements of the two adjoining crystals, *i.e.* interfacial planes, even though it uniquely describes the misorientation. Another important point: in the above example, simple topological transformations consisting of grain-boundary dissociations and mergers can transform a tetracrystal or tricrystal characterized by the $\Sigma=99$ CSL into a bicrystal with a $\Sigma99a$ grain boundary. In contrast, in the previously considered example of the $\Sigma9$–$\Sigma9$–$\Sigma9$ tricrystal, no topological transformation can generate a $\Sigma27$ grain boundary.

3. Displacement shift complete lattice of a triple junction

The triple-junction DSC lattice was introduced by Gertsman (2001*a*) as the coarsest lattice containing the three crystal lattices. It can be shown that the DSC lattice of the triple junction also contains DSC lattices of all three boundaries as sublattices.

Consider a triple junction of the three crystals defined by the lattices Λ_1, Λ_2 and Λ_3 (see Fig. 1). The DSC lattice of grain boundary GB1, $\Lambda_D^{\rm GB1}$, contains all lattice sites of Λ_1 and Λ_2. Then, the triple-junction DSC lattice, $\Lambda_D^{\rm TJ}$, can be built on Λ_3 and $\Lambda_D^{\rm GB1}$. Analogously, $\Lambda_D^{\rm TJ}$ can be built on Λ_2 and $\Lambda_D^{\rm GB2}$, and on Λ_1 and $\Lambda_D^{\rm GB3}$. Thus, all the three grain-boundary DSC lattices are sublattices of the triple-junction DSC lattice, *i.e.* their sites belong to the triple-junction DSC lattice. This can be described as follows.

Grain-boundary DSC lattices consist of vectors that can be written as sums of vectors of the two corresponding crystal lattices, *i.e.* the grain-boundary DSC vectors may be represented in following manner:

$$\mathbf{d}^{\rm GB1} = \sum_{i=1}^{3} (k_{1i}\mathbf{e}_{1i} + k_{2i}\mathbf{e}_{2i}), \tag{7a}$$

$$\mathbf{d}^{\rm GB2} = \sum_{i=1}^{3} (l_{1i}\mathbf{e}_{1i} + l_{3i}\mathbf{e}_{3i}), \tag{7b}$$

$$\mathbf{d}^{\rm GB3} = \sum_{i=1}^{3} (m_{2i}\mathbf{e}_{2i} + m_{3i}\mathbf{e}_{3i}), \tag{7c}$$

where all k, l, m are integers.

The triple-junction DSC lattice consists of vectors, which can be written as a sum of lattice vectors of Λ_1, Λ_2, Λ_3, *i.e.*

$$\mathbf{d}^{\rm TJ} = \sum_{i=1}^{3} (n_{1i}\mathbf{e}_{1i} + n_{2i}\mathbf{e}_{2i} + n_{3i}\mathbf{e}_{3i}), \tag{8}$$

where all n are integers.

It is easy to see that the set of $\mathbf{d}^{\rm TJ}$ incorporates all three sets: $\mathbf{d}^{\rm GB1}$, $\mathbf{d}^{\rm GB2}$ and $\mathbf{d}^{\rm GB3}$.

So the definition could be re-formulated as follows: the triple-junction DSC lattice is the coarsest-cell lattice containing all sites of the three crystal lattices and, as a consequence, all sites of the three grain-boundary DSC lattices.

The following property facilitates analytical determination of the triple-junction DSC lattice in every concrete case.

Triple-junction CSL–DSC lattice reciprocity. The DSC lattice of the triple junction is the reciprocal lattice of the CSL formed by the reciprocal lattices of the three crystals.

This property was surmised in Gertsman (2001*a*). It can be proven in the same way as the analogous property of the grain-boundary DSC lattice (Grimmer, 1974).

Consider again the three crystal lattices Λ_1, Λ_2, Λ_3, defined by their bases $(\mathbf{e}_{11}, \mathbf{e}_{12}, \mathbf{e}_{13})$, $(\mathbf{e}_{21}, \mathbf{e}_{22}, \mathbf{e}_{23})$ and $(\mathbf{e}_{31}, \mathbf{e}_{32}, \mathbf{e}_{33})$. The corresponding reciprocal lattices and their bases are: $\Lambda_1^*(\mathbf{e}_{11}^*, \mathbf{e}_{12}^*, \mathbf{e}_{13}^*)$, $\Lambda_2^*(\mathbf{e}_{21}^*, \mathbf{e}_{22}^*, \mathbf{e}_{23}^*)$ and $\Lambda_3^*(\mathbf{e}_{31}^*, \mathbf{e}_{32}^*, \mathbf{e}_{33}^*)$. Hereafter, the asterisk is used to indicate reciprocity. The following relationship determines the reciprocal bases:

$$\mathbf{e}_{ki}\mathbf{e}_{kj}^* = \delta_{ij}, \quad \delta_{ij} = 1 \text{ if } i = j \quad \text{and} \quad \delta_{ij} = 0 \text{ if } i \neq j. \tag{9}$$

Denote $\Lambda_C^* := {\rm CSL}(\Lambda_1^*, \Lambda_2^*, \Lambda_3^*)$. Notice that in a general case $\Lambda_C^* \neq (\Lambda_C^{\rm TJ})^*$.

We want to show that

$$\Lambda_D^{\rm TJ} = (\Lambda_C^*)^*. \tag{10}$$

We shall use the following property: a scalar product between any vectors of the direct and reciprocal lattices is an integer. With respect to our case, this can be formulated as follows: If for any vectors $\mathbf{x} \in \Lambda_C^*$ and $\mathbf{y} \in \Lambda_D^{\rm TJ}$, $\mathbf{xy}$ = integer, then

$$\Lambda_C^* \in (\Lambda_D^{\rm TJ})^*. \tag{11}$$

Vector $\mathbf{x} \in \Lambda_C^*$ if and only if

$$\mathbf{x} = \sum_{i=1}^{3} m_{1i}\mathbf{e}_{1i}^* = \sum_{i=1}^{3} m_{2i}\mathbf{e}_{2i}^* = \sum_{i=1}^{3} m_{3i}\mathbf{e}_{3i}^*. \tag{12}$$

All vectors $\mathbf{y} \in \Lambda_D$ are given by (8). Now, using (9), we can calculate

$$\mathbf{xy} = \sum_{i=1}^{3} m_{1i}\mathbf{e}_{1i}^* \sum_{i=1}^{3} n_{1i}\mathbf{e}_{1i} + \sum_{i=1}^{3} m_{2i}\mathbf{e}_{2i}^* \sum_{i=1}^{3} n_{2i}\mathbf{e}_{2i} + \sum_{i=1}^{3} m_{3i}\mathbf{e}_{3i}^* \sum_{i=1}^{3} n_{3i}\mathbf{e}_{3i}$$
$$= \sum_{i=1}^{3} (m_{1i}n_{1i} + m_{2i}n_{2i} + m_{3i}n_{3i}) = \text{integer}. \tag{13}$$

Thus, we have shown that $\Lambda_C^* \in (\Lambda_D^{\rm TJ})^*$, which is a necessary but not sufficient condition for the fulfilment of (10). At the same time, $\Lambda_D^{\rm TJ}$ contains Λ_1, Λ_2 and Λ_3 as sublattices. Then $(\Lambda_D^{\rm TJ})^* \in (\Lambda_1^*, \Lambda_2^*, \Lambda_3^*)$ and, consequently,

$$(\Lambda_D^{\rm TJ})^* \in \Lambda_C^*. \tag{14}$$

Comparing (11) and (14), we conclude that $(\Lambda_D^{\rm TJ})^* = \Lambda_C^*$. Applying the reciprocal operation, we obtain $\Lambda_D^{\rm TJ} = (\Lambda_C^*)^*$, which is relationship (10).

What is the meaning of the triple-junction DSC lattice? Recall that the grain-boundary DSC lattice is composed of all translations of one of the crystal lattices with respect to the other that leave the periodic superposition pattern unchanged (Grimmer *et al.*, 1974). That is, the DSC vectors represent such translations that retain the CSL, although the coincident sites are shifted to new positions. Such translations determine the Burgers vectors of full grain-boundary dislocations (Grimmer, 1974). The situation is more complicated for the triple-junction DSC lattice because there are more degrees of freedom in the system.

Consider the triple junction (see Fig. 1). Let us fix Λ_1 and shift Λ_2 by vector $\mathbf{s}_1$. In order to preserve the CSL of grain boundary GB1, $\mathbf{s}_1$ must be a DSC vector of GB1, *i.e.* $\mathbf{s}_1 = \mathbf{d}^{\rm GB1} \in \Lambda_D^{\rm GB1}$. However, to retain the entire superposition pattern of Λ_1, Λ_2 and Λ_3, it is also necessary to retain $\Lambda_C^{\rm GB2}$ and Λ_C^{GB3}. Two variants that satisfy this condition are possible:

(i) $$\mathbf{s}_1 = \mathbf{d}^{\rm GB1} = \mathbf{d}^{\rm GB3}, \tag{15}$$

that is, this vector belongs to $\Lambda_D^{\rm GB1}$ and $\Lambda_D^{\rm GB3}$ simultaneously; (ii) Λ_3 is shifted by $\mathbf{s}_2$ such that

$$\mathbf{s}_2 = \mathbf{d}^{\rm GB2} \in \Lambda_D^{\rm GB2} \quad \text{AND} \quad \mathbf{s}_1 - \mathbf{s}_2 = \mathbf{d}^{\rm GB3} \in \Lambda_D^{\rm GB3}. \tag{16}$$

That is, displacements at all the three boundaries are equal to the corresponding grain-boundary DSC vectors. Formally, the first variant represents a particular case of the second variant when $\mathbf{s}_2 = 0$.

It is evident that $\mathbf{s}_1$ and $\mathbf{s}_2$ belong to the triple-junction DSC lattice since any grain-boundary DSC vector is also the triple-junction DSC vector. However, not every vector of $\Lambda_D^{\rm TJ}$ retains $\Lambda_C^{\rm TJ}$ if the translation is applied only to one crystal, because in a general case translations of two crystal lattices are necessary. Then the obvious question is: what is defined by the triple-junction DSC lattice? The following section demonstrates that vectors of this lattice give the Burgers vectors of triple-junction dislocations arising from interactions between grain-boundary dislocations from contiguous boundaries.

4. Dislocation reactions at triple junctions

Only geometrical possibilities of dislocation reactions are considered in this paper without taking into account any energetic considerations.

Grain-boundary DSC lattices consist of vectors represented by equations (7), *i.e.* they can be represented as sums of the corresponding lattice vectors. The triple-junction DSC lattice consists of vectors that can be represented as sums of the three crystal lattice vectors, see equation (8).

In the particular case of an $\alpha = 1$ junction, $\Lambda_C^{\rm TJ} = \Lambda_C^{\rm GB3}$, where GB3 is the grain boundary characterized by the largest Σ. Then, $\Lambda_D^{\rm TJ} = \Lambda_D^{\rm GB3}$ and

$$\mathbf{d}^{\rm GB3} = \mathbf{d}^{\rm TJ} = \sum_{i=1}^{3} (m_{2i}\mathbf{e}_{2i} + m_{3i}\mathbf{e}_{3i}) = \sum_{i=1}^{3} (n_{1i}\mathbf{e}_{1i} + n_{2i}\mathbf{e}_{2i} + n_{3i}\mathbf{e}_{3i}). \quad (17)$$

Consider a passage of a grain-boundary dislocation from one boundary into another, *e.g.* from GB1 to GB2 (Fig. 5). In a general case, there must be a change of the Burgers vector:

$$\mathbf{b}^{\rm GB1} = \sum_{i=1}^{3} (k_{1i}\mathbf{e}_{1i} + k_{2i}\mathbf{e}_{2i}), \quad (18a)$$

$$\mathbf{b}^{\rm GB2} = \sum_{i=1}^{3} (l_{1i}\mathbf{e}_{1i} + l_{3i}\mathbf{e}_{3i}), \quad (18b)$$

$$\Delta\mathbf{b} = \mathbf{b}^{\rm GB1} - \mathbf{b}^{\rm GB2} = \sum_{i=1}^{3} [(k_{1i} - l_{1i})\mathbf{e}_{1i} - k_{2i}\mathbf{e}_{2i} + l_{3i}\mathbf{e}_{3i}]. \quad (18c)$$

In the above equations, k and l are fixed integers, unlike equations (7), where they have the meaning '*any* integer'.

Comparing (18*c*) and (8), one can notice that the residual Burgers vector is always a vector of the triple-junction DSC lattice, *i.e.*

$$\mathbf{b}^{\rm GB1} - \mathbf{b}^{\rm GB2} = \mathbf{b}^{\rm TJ} \in \Lambda_D^{\rm TJ}. \quad (19)$$

In an $\alpha = 1$ triple junction, this residual dislocation will have a Burgers vector $\mathbf{b}^{\rm TJ} \in \Lambda_D^{\rm GB3}$, so it is actually not coupled to the triple junction and may leave it for grain boundary GB3. However, in a general case of an $\alpha \neq 1$ triple junction, a residual dislocation with a Burgers vector $\mathbf{b}^{\rm TJ} \notin (\Lambda_D^{\rm GB1}, \Lambda_D^{\rm GB2}, \Lambda_D^{\rm GB3})$ may be trapped in the triple junction. Such a dislocation will be associated with the triple-junction line and its movement into any of the grain boundaries will create a grain-boundary stacking fault since it is a partial dislocation in any of the three boundaries. The following analogy can be suggested: a full grain-boundary dislocation possessing a DSC Burgers vector creates a lattice stacking fault when it is emitted from the grain boundary into the crystal.

Incidentally, (19) illustrates another definition of the triple-junction DSC lattice. Noting that the vectors of the grain-boundary DSC lattice define the geometrically possible Burgers vectors of full grain-boundary dislocations, one can see that the vectors of the triple-junction DSC lattice can be interpreted as the sum vectors of two geometrically necessary Burgers vectors of dislocations in two grain boundaries meeting at the triple junction.

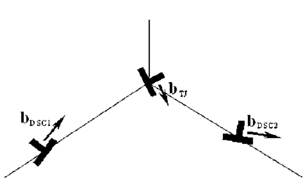

Figure 5
Passage of a grain-boundary dislocation through the triple junction.

For completeness, let us also consider a passage of a grain-boundary dislocation between GB1 (or GB2) and GB3 in an $\alpha = 1$ triple junction. Since $\Lambda_D^{\rm GB1}$ and $\Lambda_D^{\rm GB2}$ are sublattices of $\Lambda_D^{\rm TJ} = \Lambda_D^{\rm GB3}$ (see §3 above), any dislocation from GB1 or GB2 can move into GB3 without leaving residual dislocations, since their Burgers vectors are also vectors of $\Lambda_D^{\rm GB3}$. In other words, a grain-boundary dislocation approaching the triple junction from GB1 (or GB2) can be transferred to GB3 as a whole without splitting. At the reverse transmission, *i.e.* from GB3 into GB1 (or GB2), the residual Burgers vector is

$$\begin{aligned}\mathbf{b}^{\rm GB3} - \mathbf{b}^{\rm GB1} &= \sum_{i=1}^{3} [-k_{1i}\mathbf{e}_{1i} + (m_{2i} - k_{2i})\mathbf{e}_{2i} + m_{3i}\mathbf{e}_{3i}] \in \Lambda_D^{\rm TJ} \\ &= \Lambda_D^{\rm GB3}. \end{aligned} \quad (20)$$

That is, in a general case when $\mathbf{b}^{\rm GB3}$ is not a DSC vector of GB1, the original grain-boundary dislocation should split into at least two dislocations, $\mathbf{b}^{\rm GB1}$ and $\Delta\mathbf{b}$. However, the latter, the residual triple-junction dislocation, in this case is again not locked in the triple junction and may leave it for GB3.

To illustrate the above analysis, it is instructive to consider a numerical example. Grain-boundary dislocation reactions at $\alpha = 1$ triple junctions are relatively simple; see *e.g.* experimental observations and analyses of Clarebrough & Forwood (1987) as an illustration. Let us show that, in $\alpha \neq 1$ triple junctions, reactions between full grain-boundary dislocations can result in triple-junction dislocations, whose Burgers vectors are not full grain-boundary DSC vectors. Consider again the simplest $\alpha \neq 1$ junction, *i.e.* $\Sigma9$–$\Sigma9$–$\Sigma9$, in the simple cubic lattice. The triple-junction CSL in this case is characterized by $\Sigma^{\rm TJ} = 27$ (Gertsman, 2001*a*). Choose crystal lattice Λ_1 as a reference system, *i.e.* everything should be indexed in the coordinates of this crystal. The unit cell of the $\Sigma^{\rm TJ} = 27$ CSL can be described by the basis given above by (4).

The basis of the $\Sigma9$ grain-boundary CSL, $\Lambda_C^{\Sigma9}$, can be described by:

$$C_{\Sigma9} = \begin{pmatrix} -1 & -1 & 0 \\ 4 & 1 & 1 \\ 1 & 4 & 2 \end{pmatrix}. \quad (21)$$

This unit cell can be reshaped to the form given in Table 1 of Grimmer *et al.* (1974), but we have chosen the first two basis vectors in the (511) plane for an easier comparison with $C_{\Sigma^{\rm TJ}27}$ [see (4)]. From the reciprocity property (see §3), it follows that, in the primitive cubic lattice, the DSC lattice is simply the reciprocal lattice of the CSL. Then, using $A^* := (A^{-1})^T$, we obtain for the unit cells of the corresponding DSC lattices:

$$D_{\Sigma 9} = \frac{1}{9}\begin{pmatrix} -2 & -7 & 15 \\ 2 & -2 & 3 \\ -1 & 1 & 3 \end{pmatrix}. \qquad (22)$$

$$D_{\Sigma^{TJ}27} = \frac{1}{9}\begin{pmatrix} -2 & 3 & 5 \\ 2 & 0 & 1 \\ -1 & 3 & 1 \end{pmatrix}. \qquad (23)$$

Incidentally, one can check that the unit-cell volumes of Λ_C^{TJ} and Λ_D^{TJ} in this case are 27 and 1/27, correspondingly. This confirms the general property that for the triple junction $V_C = \Sigma$ and $V_D = 1/\Sigma$, as is the case for grain boundaries (see Grimmer *et al.*, 1974). The basis of Λ_D^{TJ} can be reduced to the form with the first two vectors the same as in $D_{\Sigma 9}$ by replacing the second vector in (23) by $\mathbf{e}_2 - 2\mathbf{e}_3$, *i.e.*

$$D_{\Sigma^{TJ}27} = \frac{1}{9}\begin{pmatrix} -2 & -7 & 5 \\ 2 & -2 & 1 \\ -1 & 1 & 1 \end{pmatrix}. \qquad (24)$$

Of course, the $D_{\Sigma 9}$ basis [see (22)] could also be chosen such that all its three vectors have co-prime components, but we leave it in the above form so that $\mathbf{e}_3$ lies in the [511] direction. Assume that (22) gives the basis of Λ_D^{GB1}. The two other grain boundaries in this triple junction have the same DSC lattices characteristic of the $\Sigma 9$ misorientation, but they are rotated with respect to Λ_D^{GB1}. To express their bases in the coordinate system of Λ_1, $D_{\Sigma 9}$ must be multiplied by the corresponding misorientation matrix, *i.e.* R and R^T, where

$$R = \frac{1}{9}\begin{pmatrix} 8 & 1 & 4 \\ 4 & -4 & -7 \\ 1 & 8 & -4 \end{pmatrix}. \qquad (25)$$

Thus, the DSC lattice unit cells of the three boundaries are given by the following matrices:

$$D^{GB1} = \frac{1}{9}\begin{pmatrix} -2 & -7 & 15 \\ 2 & -2 & 3 \\ -1 & 1 & 3 \end{pmatrix}, \quad D^{GB2} = \frac{1}{9}\begin{pmatrix} -2 & -6 & 15 \\ -1 & -3 & 3 \\ 2 & -3 & 3 \end{pmatrix},$$

$$D^{GB3} = \frac{1}{9}\begin{pmatrix} -1 & -7 & 15 \\ -2 & 1 & 3 \\ -2 & -2 & 3 \end{pmatrix}. \qquad (26)$$

Notice that the third basis vector is the same for all three cells because it lies along the misorientation axis.

Now assume, for example, that a grain-boundary dislocation with the Burgers vector $\mathbf{b}^{GB1} = \mathbf{e}_1 \in D^{GB1}$ goes from grain boundary GB1 into GB3 and changes its Burgers vector to $\mathbf{b}^{GB3} = \mathbf{e}_2 \in D^{GB3}$. As a result, a residual dislocation is left in the triple junction with the following Burgers vector:

$$\mathbf{b}^{TJ} = \mathbf{b}^{GB1} - \mathbf{b}^{GB3} = \tfrac{1}{9}[\bar{2}2\bar{1}] - \tfrac{1}{9}[\bar{7}1\bar{2}] = \tfrac{1}{9}[511]. \qquad (27)$$

Thus, $\mathbf{b}^{TJ} \in \Lambda_D^{TJ}$, but it is three times smaller than the DSC vector in this direction for any of the three grain boundaries [see (26)]. Hence, this dislocation cannot go into a grain boundary without generating a grain-boundary stacking fault. Only after three such dislocations are accumulated in the triple junction can the resultant dislocation leave the triple-junction line for a grain boundary as a full grain-boundary dislocation with a DSC Burgers vector.

The process considered above illustrates how triple junctions may affect grain-boundary sliding, being an obstacle for the slip transmission from boundary to boundary.

Of course, not every dislocation interaction at $\alpha \neq 1$ junctions involves trapped triple-junction dislocations. For example, in the $\Sigma 9$–$\Sigma 9$–$\Sigma 9$ junction, triple-junction DSC vectors in the (511) plane are the same as the grain-boundary DSC vectors [compare the first two column vectors in (24) and (26)]. Hence, no immobile residual triple-junction dislocation is necessary if the dislocation interaction does not involve out-of-(511)-plane Burgers vectors. Considering a general expression for dislocation transfer across the triple junction, (18*c*), one can notice that if the grain-boundary dislocation in GB2 were chosen such that $l_{1i} = k_{1i}$ $(i = 1, 2, 3)$, then the residual Burgers vector would be a DSC vector of GB3 and trapping of a residual dislocation in the triple junction could be avoided. In other words, it is always possible to find such a variant that the grain-boundary dislocation approaching the triple junction along one boundary can split into two dislocations that can leave the junction onto adjoining boundaries. Such a variant would be similar to the transmission of a dislocation from GB1 into GB2 or from GB3 into GB1 (or GB2) in an $\alpha = 1$ junction, see discussion of (19) and (20) above. However, not every reaction between grain-boundary dislocations at $\alpha \neq 1$ triple junctions can be reduced to such a situation. The example illustrated by (27) can be interpreted in the following way: meeting of the two dislocations from GB1 and GB3 at the triple junction produces a trapped triple-junction dislocation.

Summarizing, during dislocation reactions at the $\alpha = 1$ triple junction, no immobile residual triple-junction dislocation is needed.[2] Certainly, a dislocation along the triple-junction line can exist, but (purely geometrically) nothing prevents it from going into one of the adjoining grain boundaries. In the $\alpha \neq 1$ triple junction, however, some dislocation reactions may produce a triple-junction dislocation, which is trapped in the triple junction and cannot leave it without generating a stacking-fault-like defect in the grain boundary.[3] This is not to say that every dislocation reaction in an $\alpha \neq 1$ triple junction results in an immobile triple-junction dislocation, but rather to point out that no such reactions are possible in $\alpha = 1$ junctions.

The dislocation balance must include not only grain boundaries but also triple junctions. Generally, in the polycrystal there should be a net balance of lattice dislocations, grain-boundary dislocations and triple-junction dislocations. The key property for dislocation reactions could be formulated as follows: Any vector of any of the three crystal lattices

[2] It should be mentioned that the triple-junction dislocations considered in the present paper are not related to the dislocations that can arise along the triple-junction line due to different equilibrium rigid-body displacements at the adjoining grain boundaries (see *e.g.* Pond & Vitek, 1977). Those dislocations are intrinsic to the triple-junction structure, while the triple-junction dislocations considered in the present paper can be termed extrinsic.

[3] Owusu-Boahen & King (2000) surmised that dislocation reactions could be different at $\alpha = 1$ and $\alpha \neq 1$ triple junctions, though the underlying reason for the different behaviour has remained unclear.

and any vector of the three grain-boundary DSC lattices, *i.e.* any Burgers vector of lattice or grain-boundary dislocations can be decomposed into the basis vectors of the corresponding triple-junction DSC lattice.

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