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Geometrical theory of triple junctions of CSL boundaries

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When three grain boundaries having misorientations generating coincidence site lattices (CSLs) meet at a triple junction, a common (triple-junction) CSL is formed. A theory is developed as a set of theorems establishing the relationships between the geometrical parameters of the grain-boundary and triple-junction CSLs. Application of the theory is demonstrated in detail for the case of the cubic crystal system. It is also shown how the theory can be extended to an arbitrary crystal lattice.

1. Introduction

Triple junctions of grains (and, consequently, of grain boundaries) have been known to researchers ever since it was realised that most crystalline materials exist in the polycrystalline form. Yet only recently triple junctions have attracted a considerable amount of attention and it has been recognized that they are not just geometrical locations where grain boundaries meet but that the triple junction should be considered as a separate structural element of polycrystals that can considerably influence material properties [see *e.g.* the *Interface Science* Special Issue on Triple Junctions (Gottstein *et al.*, 1999)]. Progress in this field is hindered, however, by the lack of an accredited crystallographic theory that would help analyze experimental data and could serve as a framework for phenomenological models. In the case of grain boundaries, the coincidence site lattice theory, CSL (*e.g.* Grimmer *et al.*, 1974), has provided such a crystallogeometrical framework. Even though considerable difficulties exist in direct correlation of the CSL approach with physical properties of grain boundaries (see *e.g.* Sutton & Balluffi, 1987 and Gertsman & Szpunar, 1999), the CSL model has proven to be an extremely useful tool in advancing our understanding of the grain-boundary structure and properties. The present work is an effort to provide such a tool for triple junctions. In this paper, we will be dealing only with the triple junctions of unstressed crystals. Very interesting junction structures can be formed if elastic distortions in the grains are allowed, which could lead *e.g.* to junction disclinations (see Dimitrakopulos *et al.*, 1999 and Gertsman, 1999). However, this does not change the fact that a geometric theory of unstressed triple junctions can serve as a basis for analyzing triple-junction defects just as the perfect crystal lattice is a framework for analyzing crystal-lattice defects. The reason the crystallographic approach to triple junctions lags behind the grain-boundary crystallographic theories may be that the object is much more complex. King (1999) has shown that, in a general case, the triple junction has 11 macroscopic and 15 microscopic degrees of freedom as compared to 5 and 3, respectively, for the grain boundary. Microscopic degrees of freedom are not the subject of geometric theories and we do not consider grain-boundary planes in this study, either. Nevertheless, we are still left with six rotational degrees of freedom for the triple junction, while the grain boundary has only three.

The paper is constructed in the following way: §2 gives a very brief overview of what has been known to date on the issue. The theory is formulated as a set of theorems for the cubic crystal system in §3. Application of the theory to describe geometrical parameters of triple junctions of grains with the cubic lattice is described in §4 and some special cases are discussed in §5. Finally, §6 demonstrates how the theory can be generalized for an arbitrary crystal lattice.

2. Background

The particular class of triple junctions we are considering in the current work are those where three CSL boundaries meet. It has been recognized for quite some time that in such a case a common lattice of sites common to all three adjoining lattices (triple-junction CSL) should exist and that there must be a relationship among the parameters of the three grain-boundary CSLs (*e.g.* Andreeva *et al.*, 1982; Kopezky & Fionova, 1982; Perevezentsev *et al.*, 1982). The commonly accepted parameter characterizing a CSL is the multiplicity factor, the so-called reciprocal density of coincident sites, Σ (*e.g.* Grimmer *et al.*, 1974). A geometrical theory must give the Σ combination rule for the boundaries comprising the triple junction as well as an algorithm to calculate Σ of the triple-junction CSL, which we denote as Σ^{TJ}.

There is a widely spread misconception concerning the Σ combination rule: in most publications, it is assumed that in the triple junction one of the Σ's (*e.g.* Σ_3) is always greater than the other two and the formula is

$$\Sigma_3 = \Sigma_1 \Sigma_2, \tag{1}$$

where the subscripts refer to the grain boundaries. However, this formula reflects only a particular solution of the relationship. General solutions for the cubic system were suggested in the Russian (Andreeva *et al.*, 1982; Kopezky & Fionova, 1982) and Japanese (Miyazawa *et al.*, 1983) literature, but have gone almost unnoticed.

The former approach can be summarized as follows. The rotation matrix for a CSL misorientation between two cubic crystal lattices can be represented as

$$R = \frac{1}{\Sigma}\{a\} = \frac{1}{\Sigma}\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}, \qquad (2)$$

where all a_{ij} are co-prime (*i.e.* having no common divisor except 1) integers. The formula for the Σ combination rule at a CSL triple junction can be written as

$$\Sigma_3 = \Sigma_1 \Sigma_2 / \alpha, \qquad (3)$$

where α is the greatest common divisor (g.c.d.) of the matrix $\{b\} = \{a\}_1\{a\}_2$.

On the other hand, Miyazawa *et al.* (1983) suggested that

$$\Sigma_3 = \Sigma_1 \Sigma_2 / \beta^2, \qquad (4)$$

where β is a common divisor of Σ_1 and Σ_2.

It will be shown in the next section that the two statements are both true, which implies that the g.c.d. of the elements of the matrix $\{b\}$ is always the square of a common divisor of Σ_1 and Σ_2.

It should be noted, however, that in the above-cited papers it was still implied that in the triple junction one of the α values is always equal to 1, and the proposed relationships were designed so that the general formula be applicable to all boundaries in the junction, not just for the calculation of the largest Σ. To the best of the author's knowledge, it had not been until 1995 when it was first shown (Gertsman & Tangri, 1995) that triple junctions where none of the α's are equal to 1 do exist. Hereafter, we shall call such a triple junction '$\alpha \neq 1$ junctions'. That paper gives a $\Sigma 9$–$\Sigma 9$–$\Sigma 9$ junction as an example. The next year, the possibility of a $\Sigma 9$–$\Sigma 9$–$\Sigma 9$ junction was shown by Dimitrakopulos & Karakostas (1996) on the basis of symmetry considerations, but they still wrote that in this case '*the well known CSL multiplication rule* [meaning formula (1)] *is not valid*'. The same year, Miyazawa *et al.* (1996) expanded their earlier hypothesis and demonstrated the possibility of many $\alpha \neq 1$ triple junctions in the cubic crystal system. However, they offered the proof of formula (4) only for a particular case and conjectured that it was generally applicable on the basis of a limited number of numerical calculations. Recently, Owusu-Boahen & King (2000) have suggested that, if $\alpha \neq 1$, the triple junction may have some special properties. In their analysis, they have implied that such junctions have all three $\alpha \neq 1$, even though they did not mention this explicitly in their paper. Of course, in every triple junction $\alpha \neq 1$ for at least one of the boundaries. So, we emphasize that the term '$\alpha \neq 1$ junction' refers only to the cases when none of the α's are equal to 1.

The question about the coincident site density of the triple-junction CSL has remained moot. Perevezentsev *et al.* (1982) showed that $\Sigma^{\rm TJ} = \max(\Sigma_1, \Sigma_2, \Sigma_3)$, but they implied that formula (1) was always valid; therefore, their solution refers only to $\alpha = 1$ junctions. Miyazawa *et al.* (1996) put forth a conjecture that $\Sigma^{\rm TJ} = (\Sigma_1\Sigma_2\Sigma_3)^{1/2}$, but they did not offer any proof of this relationship.

3. Primary theorems

Even though equation (3) first appeared almost two decades ago, to the best of the author's knowledge a thorough proof of it has never been published. Perhaps it looked obvious to the original authors; however, the Σ combination rule is still continuing to be quoted simply as $\Sigma_3 = \Sigma_1\Sigma_2$. Therefore, it seems necessary to show how the result can be obtained.

Theorem 1. Σ combination rule for the cubic crystal system. Let two of the boundaries in the triple junction have CSL misorientations with the reciprocal densities of coincident sites Σ_1 and Σ_2. Rotation matrices of these misorientations can be represented in the form of equation (2), *i.e.*

$$R_1 = \frac{1}{\Sigma_1}\{a_{ij}\}_1 \quad \text{and} \quad R_2 = \frac{1}{\Sigma_2}\{a_{ij}\}_2, \qquad (5)$$

where $\{a_{ij}\}$ are integral irreducible matrices. Then the third grain boundary in the junction has a CSL misorientation described by

$$\Sigma_3 = \Sigma_1\Sigma_2/\alpha_{12}, \qquad (6)$$

where α_{12} is the g.c.d. of the matrix

$$\{b_{ij}\} = \{a_{ij}\}_1\{a_{ij}\}_2. \qquad (7)$$

For three boundaries meeting at a triple junction, the following equation is valid when grain orientations are determined in the same reference system:

$$R_1R_2R_3 = I, \qquad (8)$$

where I is the identity matrix.

From (8),

$$R_1R_2 = R_3^{-1}. \qquad (9)$$

The inverse matrix R_3^{-1} describes an equivalent variant of the same misorientation as R_3, *i.e.* the third misorientation can be found as a product of the first two misorientations. It actually does not matter which matrix is considered to be direct and which inverse. Therefore, formula (9) is often written as

$$R_1R_2 = R_3. \qquad (9a)$$

In the cubic crystal system, the rotation matrix is orthonormal; therefore, the inverse and transpose matrices are the same, *i.e.* $R^{-1} = R^T$.

In the expanded form, equation (9) is expressed as

$$\frac{1}{\Sigma_1}\{a_{ij}\}_1\frac{1}{\Sigma_2}\{a_{ij}\}_2 = \frac{1}{\Sigma_3}\{a_{ij}\}_3^T. \qquad (10)$$

Multiplication of the left-hand side of (10) gives

$$\frac{1}{\Sigma_1}\{a_{ij}\}_1 \frac{1}{\Sigma_2}\{a_{ij}\}_2 = \frac{1}{\Sigma_1\Sigma_2}\{b_{ij}\}. \quad (11)$$

The $\{b_{ij}\}$ matrix elements are calculated as

$$b_{ij} = (a_{i1})_1(a_{1j})_2 + (a_{i2})_1(a_{2j})_2 + (a_{i3})_1(a_{3j})_2. \quad (12)$$

Because R_1 and R_2 are CSL rotations, all $(a_{ij})_1$ and $(a_{ij})_2$ are integers. Then all b_{ij} are integers as well. Therefore, all components of matrix R_3^{-1} (and, consequently, of R_3) are rational and it describes a CSL rotation. Components of each of the matrices $\{a_{ij}\}_1$ and $(a_{ij})_2$ do not have common divisors. This does not, however, mean that all b_{ij} do not have a common divisor. Simply speaking, it is possible to construct nine integers having a common divisor out of two sets of nine co-prime integers according to (12). If matrix $\{b_{ij}\}$ is irreducible, then from (10) and (11) it follows that $b_{ij} = \{a_{ij}\}_3^T$ and $\Sigma_3 = \Sigma_1\Sigma_2$. If the components of matrix $\{b_{ij}\}$ do have a common divisor, α_{12}, then from (10) and (11) we obtain $\{a_{ij}\}_3^T = \{b_{ij}\}/\alpha_{12}$ and $\Sigma_3 = \Sigma_1\Sigma_2/\alpha_{12}$.

Corollary. *α combination rule*. For a triple junction of three CSL boundaries between cubic lattice crystals,

$$\alpha_{12}\alpha_{13}\alpha_{23} = \Sigma_1\Sigma_2\Sigma_3. \quad (13)$$

This simply follows from

$$\alpha_{12}\Sigma_3 = \Sigma_1\Sigma_2, \quad \alpha_{13}\Sigma_2 = \Sigma_1\Sigma_3, \quad \alpha_{23}\Sigma_1 = \Sigma_2\Sigma_3. \quad (14)$$

Possible values of α can be found using the following theorem.

Theorem 2. *α theorem*. In the cubic crystal system, α_{12} is the square of a common divisor of Σ_1 and Σ_2 (correspondingly, $\Sigma_1|\alpha_{13}^{1/2}$, $\Sigma_3|\alpha_{13}^{1/2}$ and $\Sigma_2|\alpha_{23}^{1/2}$, $\Sigma_3|\alpha_{23}^{1/2}$).[1]

As mentioned in §2, this proposition was first put forward by Miyazawa *et al.* (1983). Later, Miyazawa *et al.* (1996) proved it for a particular case when both generating misorientations can be represented by 180° rotations about a common axis and from numerical calculations conjectured it to be valid in a general case. Here we give a more general proof of the theorem.

First, let us show that in the cubic crystal system α is a square of an odd integer. That α is odd simply follows from the fact that all three Σ's in formula (3) are odd integers. To show that it is a square, let us use the vector-quaternion description of misorientations (Gertsman, 1989, 1990). Any CSL misorientation can be described by a Rodrigues–Gibbs vector

$$\mathbf{G} = \kappa[k, l, m]/n \quad (15)$$

or quaternion

$$(k, l, m, n), \quad (16)$$

where k, l, m, n are co-prime integers. For the cubic system, $\kappa = 1$.

[1] Notation $a|b$ means that integer a is divisible by integer b.

This quaternion describes the rotation about the axis $[k, l, m]$ by the angle θ such that

$$\tan^2(\theta/2) = (k^2 + l^2 + m^2)/n^2 \quad (17)$$

and

$$\Sigma \text{ is the greatest odd factor of } (k^2 + l^2 + m^2 + n^2). \quad (18)$$

Consider a product of two CSL misorientations. From the multiplication law for orthonormal quaternions (*e.g.* Grimmer, 1974*a*), one obtains

$$(k_1, l_1, m_1, n_1)(k_2, l_2, m_2, n_2) = (K, L, M, N), \quad (19)$$

where

$$\begin{aligned} K &= k_1n_2 + n_1k_2 + l_1m_2 - m_1l_2 \\ L &= m_1k_2 - k_1m_2 + n_1l_2 + l_1n_2 \\ M &= k_1l_2 - l_1k_2 + n_1m_2 + m_1n_2 \\ N &= n_1n_2 - k_1k_2 - l_1l_2 - m_1m_2. \end{aligned} \quad (19a)$$

Even though both generating quaternions contain co-prime coefficients, the product quaternion may still be reducible. Let β be the greatest common odd divisor of (K, L, M, N). Then,

$$\Sigma_3 \text{ is the greatest odd factor of } (K^2 + L^2 + M^2 + N^2)/\beta^2. \quad (20)$$

From (19*a*), it is easy to obtain by direct calculation that

$$K^2 + L^2 + M^2 + N^2 = (k_1^2 + l_1^2 + m_1^2 + n_1^2)(k_2^2 + l_2^2 + m_2^2 + n_2^2). \quad (21)$$

Using (18), (20) and (21), we obtain

$$\Sigma_3 = \Sigma_1\Sigma_2/\beta^2. \quad (22)$$

Thus, we have proven that in any event α in formula (3) is a square of an odd integer. Instead of theorem 1, which deals with rotation matrices, we can now formulate the corresponding theorem for the cubic quaternions: $\Sigma_3 = \Sigma_1\Sigma_2/\beta^2$, where β is the greatest common odd divisor of the quaternion produced by multiplication of two quaternions describing the two generating CSL misorientations.

The matrix formulation can be obtained directly from the quaternion formulation. The rotation matrix corresponding to orthogonal quaternion (K, L, M, N) is represented by (*e.g.* Korn & Korn, 1983)

$$1/(K^2 + L^2 + M^2 + N^2) \times \begin{pmatrix} K^2 - L^2 - M^2 + N^2 & 2(KL - MN) & 2(KM + LN) \\ 2(KL + MN) & -K^2 + L^2 - M^2 + N^2 & 2(LM - KN) \\ 2(KM - LN) & 2(LM + KN) & -K^2 - L^2 + M^2 + N^2 \end{pmatrix}. \quad (23)$$

Therefore, if β is the greatest common odd divisor of the quaternion (K, L, M, N), then $\beta^2 = \text{g.c.d.}\{b_{ij}\}$. We have left the matrix formulation of the Σ combination rule in the current paper since it allows easier extension to an arbitrary crystal system.

Now let us return to the proof of the α theorem. From (14) using (22), we obtain:

$$\Sigma_1 = \Sigma_2\Sigma_3/\alpha_{23} = \Sigma_1\Sigma_2^2/\alpha_{23}\beta^2, \quad (24)$$
$$\Sigma_2 = \Sigma_1\Sigma_3/\alpha_{13} = \Sigma_1^2\Sigma_2/\alpha_{13}\beta^2. \quad (25)$$

From (24) and (25), it follows that

$$\alpha_{13} = (\Sigma_1/\beta)^2, \quad \alpha_{23} = (\Sigma_2/\beta)^2. \quad (26)$$

Since all α's must be integer, then $\Sigma_1|\beta$ and $\Sigma_2|\beta$. That is, β is a common divisor of Σ_1 and Σ_2.

Corollary. In the cubic system, the case is always that

$$\Sigma_1 = pq, \quad \Sigma_2 = pr, \quad \Sigma_3 = qr, \quad (27)$$

where p, q, r are positive integers.

Proof. Proof is simple: Let $\alpha_{12} = p^2$, then from Theorem 2 $\Sigma_1 = pq$ and $\Sigma_2 = pr$, and from (6) $\Sigma_3 = qr$.

As mentioned in §2, that three CSL misorientations produce a common CSL has been evident to researchers for quite some time. However, the question remains about the reciprocal density of coincident sites, $\Sigma^{\rm TJ}$, in the triple-junction CSL. Perevezentsev *et al.* (1982) found that $\Sigma^{\rm TJ} = \max(\Sigma_1, \Sigma_2, \Sigma_3)$, but they implicitly assumed that $\alpha = 1$ always for one of the boundary pairs. More recently, Miyazawa *et al.* (1996) put forward a conjecture that $\Sigma^{\rm TJ} = (\Sigma_1\Sigma_2\Sigma_3)^{1/2}$, but they did not offer any proof of it. The next theorem shows how this result can be derived.

Theorem 3. Σ^{TJ} *theorem*. Superposition of three cubic lattices, misoriented in such a way that each pair of the lattices creates a CSL, generates a triple-junction CSL with the multiplicity factor

$$\Sigma^{\rm TJ} = (\Sigma_1\Sigma_2\Sigma_3)^{1/2}. \quad (28)$$

Lemma. Consider two superimposed misoriented crystal lattices, L_1 and L_2, forming a CSL with the reciprocal density of coincident sites Σ. The coordinate origin is the same for L_1 and L_2 and is placed at a lattice site of both lattices. The spacing between coincident sites along any rational direction $\mathbf{x}$ in either of the crystal lattices is no larger than Σx, where x is the spacing between crystal lattice sites along $\mathbf{x}$.

The spacing between lattice sites along any crystal direction in L_1 is defined by the length x of the vector $\mathbf{x}_1$ having three co-prime integer components. The direction in L_2, coinciding with $\mathbf{x}_1$, can be determined by the vector $\mathbf{x}_2 = R\mathbf{x}_1$, which has the same length x. For a CSL misorientation $R = \{a\}/\Sigma$, where $\{a\}$ is an integral matrix. Therefore, vector $\Sigma\mathbf{x}_2$ will always have integer components, *i.e.* it ends at a lattice site of L_2. This vector also ends at a lattice site of L_1, because its length is equal to Σx and there is an integer number of translations $\mathbf{x}_1$ within its length. Thus, this vector defines a coincident site of the two crystal lattices. Of course, intermediate coincident sites are also possible if the components of $\Sigma\mathbf{x}_2$ have common divisors, but there are always coincident sites with the spacing of Σx. Moreover, since the components of $\{a\}$ are co-prime integers, it is always possible to choose $\mathbf{x}_1$ such that the components of $\Sigma\mathbf{x}_2$ are co-prime. Thus, if the spacing of coincident sites along all possible rational directions in the crystal lattice is no larger than Σ times spacings of the crystal lattice sites in the corresponding directions, then Σ is the reciprocal density of coincident sites.

Now, returning to the main theorem, consider three superimposed cubic crystal lattices, L_1, L_2 and L_3, such that each pair of the lattices produces a CSL (grain-boundary CSL). Denote the corresponding densities of coincident sites: Σ_1 for the CSL$_1$ between L_1 and L_2, Σ_2 for the CSL$_2$ between L_2 and L_3, and Σ_3 for the CSL$_3$ between L_1 and L_3. The coordinate origin is the same for L_1, L_2 and L_3 and is placed at a lattice site in each of the lattices. Choose a coordinate system of L_1 and a rational direction in it, $\mathbf{x}$, defined by the vector $\mathbf{x}_1$ having three co-prime integer components. Denote the length of $\mathbf{x}_1$ as x. Obviously, the spacings along $\mathbf{x}$ of coincident sites of the three grain-boundary CSLs are no larger than Σ_1x, Σ_2x, Σ_3x, correspondingly. A common CSL (triple-junction CSL) for all three crystal lattices exists if there are sites common for CSL$_1$, CSL$_2$ and CSL$_3$. In the $\mathbf{x}$ direction, the spacing of the triple-junction CSL sites, $\Sigma^{\rm TJ}x$, must contain integer numbers of coincident site spacings of all the three grain-boundary CSLs in this direction. Recall from the corollary to theorem 2 that $\Sigma_1 = pq$, $\Sigma_2 = pr$ and $\Sigma_3 = qr$. It is evident that

$$\Sigma^{\rm TJ} = pqr \quad (29)$$

satisfies the condition of the existence of a lattice of sites common to all three grain-boundary CSLs and, as a consequence, to all three crystal lattices.

In the case $\alpha_{12} = 1, p = 1$ and $\Sigma^{\rm TJ} = \Sigma_3 = qr$. Thus, indeed, if one of the α's is equal to 1, $\Sigma^{\rm TJ} = \max(\Sigma_1, \Sigma_2, \Sigma_3)$.

Is it possible that there exists a triple-junction CSL with a multiplicity factor smaller than that determined by (29)? Suppose it is so and $\Sigma^{\rm TJ} = pqr/t$, where t is a positive integer. First, consider the case when all three grain-boundary CSLs are not the same and do not completely coincide. For any direction $\mathbf{x}$, the ratios of the spacings $\Sigma^{\rm TJ}x/\Sigma_ix$ must be integers. Then, all three Σ values for the grain-boundary CSLs must be divisible by t. Therefore, the triple-junction CSL of three grain-boundary CSLs, characterized by Σ_1, Σ_2 and Σ_3, can also be produced by superposition of three grain-boundary CSLs with $\Sigma_1' = \Sigma_1/t$, $\Sigma_2' = \Sigma_2/t$ and $\Sigma_3' = \Sigma_3/t$. That would mean that three given crystal orientations could produce a different triplet of CSLs congruent with CSL$_1$, CSL$_2$ and CSL$_3$. Hence, $t \equiv 1$.

In principle, however, one other case is possible where all three ratios $\Sigma^{\rm TJ}/\Sigma_i$ are integer, but $\Sigma^{\rm TJ}$ is not determined by (29). This is the case when $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3$. Since the ratios $\Sigma^{\rm TJ}x/\Sigma_ix$ must be the same for all possible directions $\mathbf{x}$, then all three grain-boundary CSLs must completely coincide and not just have the same Σ values describing different CSLs. As such, all three misorientations between the crystal lattices must be the same and, since their sum must produce the full rotation, they can all be described as 120° rotations about a

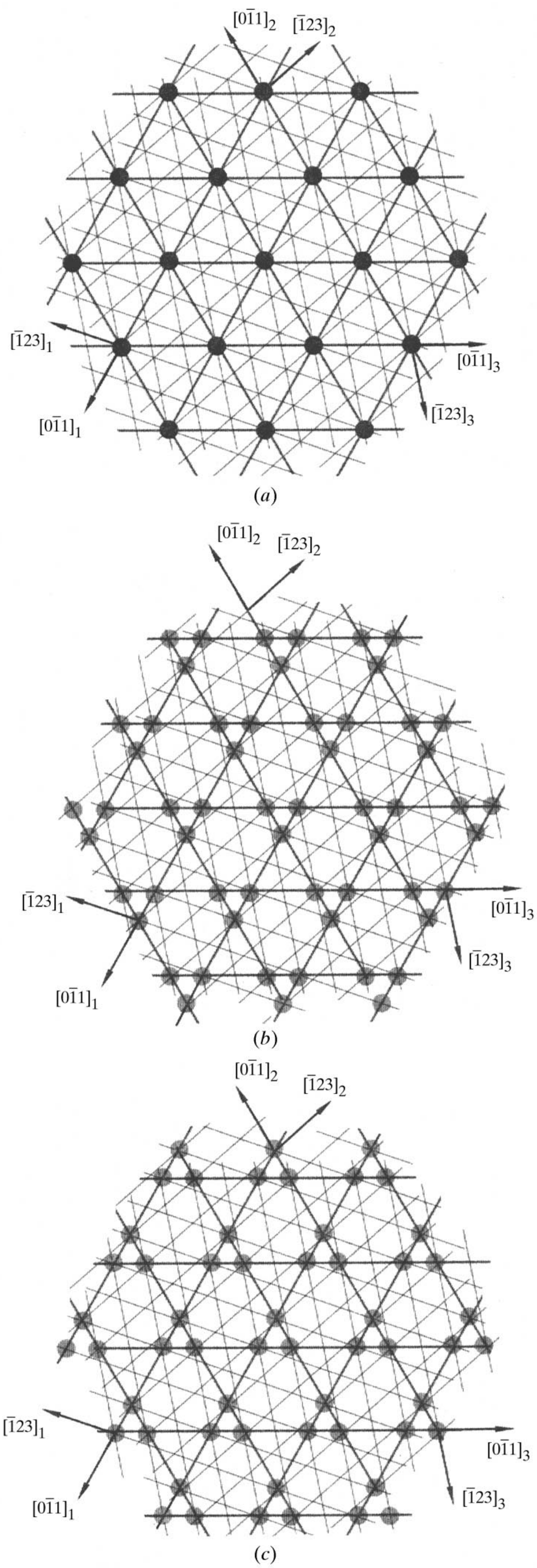

Figure 1
Superposition of three misoriented simple cubic lattices. The projection direction is [511]. Three layers of lattice sites are shown: (*a*) at zero height, (*b*) at height $3^{-1/2}$, and (*c*) at height $2 \times 3^{-1/2}$. Black circles indicate the lattice sites common for all three crystal lattices, while gray circles denote the lattice sites common only to pairs of the crystal lattices.

common axis.[2] From the vector–quaternion description of misorientations (Gertsman, 1989, 1990), it follows that a misorientation by 120° about an axis [*klm*] generates a CSL only if the following condition is met [see equation (17) above]:

$$(k^2 + l^2 + m^2)/n^2 = 3, \qquad (30)$$

where *k*, *l*, *m* and *n* are integers.

The lowest-index[3] axis satisfying this equation is [511], and the 120° [511] rotation indeed produces the CSL with $\Sigma = 9$. Fig. 1 shows three superimposed lattices with the $\Sigma = 9$ misorientation between each pair. One can see that in the plane of the drawing (see Fig. 1*a*) every third lattice site is common for each of the three crystal lattices. However, such a situation takes place only in every ninth (511) plane. Each pair of crystal lattices also has coincident sites in every third (511) plane, but these are not common for all the three lattices (see Figs. 1*b* and 1*c*). Hence, in this example all three grain-boundary CSLs have $\Sigma = 9$, but $\Sigma^{\rm TJ} = 27$ [which, incidentally, satisfies formula (29)]. From this consideration, it is evident that, in general, $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3$ only if the rotation axis [*klm*] is perpendicular to a mirror symmetry plane in the crystal lattice. One can easily check that (30) does not have integer solutions for rotation axes [100] and [110]. Therefore, the case $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3$ is impossible in the cubic system. The curious reader can check that the next (after $\Sigma = 9$) 120° rotation generating a CSL is about the [751] axis, which gives $\Sigma 25b$. Superposition of three $\Sigma 25b$ CSLs produces a situation similar to that with the three $\Sigma 9$ CSLs.

Thus, we have shown that in the cubic system we always have $\Sigma^{\rm TJ} = pqr$, which, taking into account the corollary to theorem 2, is equivalent to (28). Other useful relationships that follow from this one are

$$\Sigma^{\rm TJ} = \frac{\Sigma_1 \Sigma_2}{\alpha_{12}^{1/2}} = \frac{\Sigma_1 \Sigma_3}{\alpha_{13}^{1/2}} = \frac{\Sigma_2 \Sigma_3}{\alpha_{23}^{1/2}}. \qquad (31)$$

4. Numerical examples of $\alpha \neq 1$ triple junctions in the cubic crystal system

The relationships described in the previous section allow calculation of any possible combination of CSL misorientations at triple junctions of crystals belonging to the cubic system. We will not consider here trivial cases when one of the α values is equal to 1 and the Σ values are related through formula (1). Only the results for those junctions where two of the Σ values do not exceed 30 are presented in the following tables.

Table 1 gives all possible $\alpha \neq 1$ triple junctions where all three boundary misorientations can be described as rotations about an axis common for all three crystals. Of course, in a general case for a crystal lattice to be brought into coincidence

[2] Excluding the trivial case $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3 = 1$. This means that all three crystal lattices completely coincide and the rotations between them are just symmetry operations for the given crystal system.
[3] Excluding [111], since 120° [111] simply describes a symmetry operation in the cubic system.

Table 1
$\alpha \neq 1$ triple junctions when all three boundaries have a common rotation axis.

Σ_1	Σ_2	Σ_3	$\theta_1[uvw]_1$	$\theta_2[uvw]_2$	$\theta_3[uvw]_3$	α_{1-2}	α_{1-3}	α_{2-3}	Σ^{TJ}
9	9	9	120° [511]	120° [511]	120° [511]	9	9	9	27
			90° [221]	90° [221]	180° [221]				
9	15	15	123.7° [321]	86.2° [321]	150.1° [321]	9	9	25	45
			160.8° [531]	99.6° [531]	99.6° [531]				
9	21*a*	21*b*	152.7° [410]	79.0° [410]	128.2° [410]	9	9	49	63
			152.7° [322]	128.2° [322]	79.0° [322]				
9	27*a*	27*b*	180° [411]	70.5° [411]	109.5° [411]	9	9	81	81
			120° [511]	180° [511]	60° [511]				
15	15	25*a*	134.4° [711]	134.4° [711]	91.1° [711]	9	25	25	75
15	15	25*b*	113.6° [421]	113.6° [421]	132.8° [421]	9	25	25	75
			134.4° [551]	134.4° [551]	91.1° [551]				
15	21*a*	35*a*	137.2° [510]	103.8° [510]	119.1° [510]	9	25	49	105
15	21*a*	35*b*	165.2° [553]	113.9° [553]	81.0° [553]	9	25	49	105
15	21*b*	35*a*	99.6° [531]	80.4° [531]	180° [531]	9	25	49	105
			165.2° [731]	113.9° [731]	81.0° [731]				
15	21*b*	35*b*	113.6° [421]	180° [421]	66.4° [421]	9	25	49	105
			137.2° [431]	103.8° [431]	119.1° [431]				
15	27*a*	45*a*	137.2° [510]	157.8° [510]	65.0° [510]	9	25	81	135
15	27*a*	45*b*	159.0° [520]	94.2° [520]	106.8° [520]	9	25	81	135
15	27*b*	45*a*	159.0° [432]	94.2° [432]	106.8° [432]	9	25	81	135
15	27*b*	45*c*	117.8° [311]	79.3° [311]	162.9° [311]	9	25	81	135
			137.2° [431]	157.8° [431]	65.0° [431]				
21*a*	21*a*	49*a*	98.2° [111]	98.2° [111]	163.6° [111]	9	49	49	147
			141.8° [111]	141.8° [111]	76.4° [111]				
21*b*	21*b*	49*a*	124.9° [441]	124.9° [441]	110.3° [441]	9	49	49	147
21*b*	21*b*	49*b*	124.9° [522]	124.9° [522]	124.9° [522]	9	49	49	147
21*b*	21*b*	49*c*	58.4° [210]	154.8° [210]	146.8° [210]	9	49	49	147
			141.8° [751]	141.8° [751]	76.4° [751]				
21*a*	27*a*	63*b*	113.9° [553]	95.3° [553]	150.8° [553]	9	49	81	189
21*a*	27*b*	63*a*	167.5° [911]	122.5° [911]	70.0° [911]	9	49	81	189
21*b*	27*a*	63*a*	144.0° [611]	114.0° [611]	101.9° [611]	9	49	81	189
21*b*	27*b*	63*b*	154.8° [210]	35.4° [210]	169.8° [210]	9	49	81	189
			144.0° [532]	114.0° [532]	101.9° [532]				
21*b*	27*b*	63*c*	113.9° [731]	95.3° [731]	150.8° [731]	9	49	81	189
25*a*	25*b*	25*b*	180° [430]	90° [430]	90° [430]	25	25	25	125
25*b*	25*b*	25*b*	120° [751]	120° [751]	120° [751]	25	25	25	125
27*a*	27*a*	81*c*	146.4° [755]	146.4° [755]	67.1° [755]	9	81	81	243
27*b*	27*b*	81*a*	131.8° [542]	131.8° [542]	96.4° [542]	9	81	81	243
27*b*	27*b*	81*c*	109.5° [411]	109.5° [411]	141.1° [411]	9	81	81	243
			146.4° [771]	146.4° [771]	67.1° [771]				

with itself it is not necessary that three rotations be about the same axis. The cases when three constituent misorientations cannot be described as rotations about a common axis are presented in Table 2. Misorientations in Table 2 are chosen such that $\theta_1[uvw]_1 = 180^\circ\,[uvw]_1$ and $\theta_2[uvw]_2 = 180^\circ\,[uvw]_2$. In this case, $[uvw]_3 = [uvw]_1 \times [uvw]_2$ and $\theta_3 = 2(\measuredangle[uvw]_1, [uvw]_2)$.

It should be mentioned that relationships (27) provide only the necessary condition, but their fulfilment is not enough for the triple junction to be in fact possible. To find whether a certain combination can exist, it is necessary to directly check the misorientation multiplication in the matrix, vector-quaternion or any other form (whichever one prefers). As an example, Table 3 lists potential combinations for the $\alpha \neq 1$ triple junctions, which are impossible.

Tables 1 and 2 are somewhat similar to Table 1 of Miyazawa *et al.* (1996). However, despite a certain overlap of the present results with the result computed by Miyazawa *et al.*, the following differences are worth mentioning. The data in their table were calculated for the cases when all three Σ values were capped at $\Sigma = 49$. Also, their choices of the grain-boundary misorientation descriptions are unclear. Besides, checking the variants with $\Sigma_1, \Sigma_2 > 30$ shows that a couple of possible variants are missing: $\Sigma 9$–$\Sigma 21b$–$\Sigma 21b$ and $\Sigma 15$–$\Sigma 21b$–$\Sigma 35$.

5. Discussion

One of the difficulties in triple-junction studies has been the lack of convenient and simple categorization of such objects. Existence of the triple-junction CSL provides a possible means for such a classification. Certainly, as with grain boundaries, the Σ description of triple junctions may simply be a classification of convenience and we are not hinting at any link of physical properties of the junction with the magnitude of Σ^{TJ}. Nevertheless, it is remarkable that such a complex object can be characterized by a single scalar parameter.

The proposed geometric theory allows singling out at least one class of triple junctions, namely $\alpha \neq 1$ junctions. At present, we do not know how frequent such junctions are in real polycrystals. At least, the analysis of Table 1 of Miyazawa *et al.* (1996) shows that, if Σ is capped for all constituent grain boundaries, then $\alpha \neq 1$ triple junctions quickly become predominant among the junctions of CSL boundaries. Of course, if Σ_3 were kept uncapped, then $\alpha \neq 1$ triple junctions would be in the minority. However, 'rare' does not necessarily mean 'unimportant'. Recently, Owusu-Boahen & King (2000) suggested that $\alpha \neq 1$ triple junctions may have special properties, different from those of $\alpha = 1$ junctions, in particular with regard to dislocation transmission between grain boundaries meeting at the junction. Their hypothesis is based on the consideration of the displacement shift complete (DSC) lattice, which can be defined as the coarsest lattice containing the two grain lattices as sublattices (see *e.g.* Grimmer *et al.*, 1974 and Sutton & Balluffi, 1995). Owusu-Boahen & King have demonstrated graphically that in $\alpha = 1$ junctions the DSC lattice of the boundary with the largest Σ contains DSC lattices of the other two boundaries as sublattices.[4] This is actually a corollary from theorem 3, which shows that, when $\alpha_{12} = 1$, CSL$_1$ and CSL$_2$

[4] It is noteworthy that this statement was proven theoretically by Perevezentsev *et al.* (1982) who thought it was generally valid since they considered only $\alpha = 1$ triple junctions.

Table 2
$\alpha \neq 1$ triple junctions when constituent grain boundaries do not have a common rotation axis.

Σ_1	Σ_2	Σ_3	$\theta_1[uvw]_1$	$\theta_2[uvw]_2$	$\theta_3[uvw]_3$	α_{1-2}	α_{1-3}	α_{2-3}	$\Sigma^{\rm TJ}$
9	21*b*	21*b*	180° [221]	180° [142]	58.4° $[0\bar{1}2]$	9	9	49	63
27*b*	27*b*	9	180° [721]	180° $[27\bar{1}]$	120° [115]	81	9	9	81
15	27*a*	45*c*	180° [521]	180° [115]	130.1° $[3\bar{8}1]$	9	25	81	135
15	27*b*	45*b*	180° [521]	180° [172]	117.1° $[\bar{1}\bar{3}11]$	9	25	81	135
21*a*	21*b*	49*b*	180° [541]	180° $[\bar{2}\bar{4}\bar{1}]$	49.2° $[0\bar{1}4]$	9	49	49	147
21*a*	21*b*	49*c*	180° [541]	180° [214]	105.4° $[5\bar{6}\bar{1}]$	9	49	49	147
21*a*	27*b*	63*c*	180° [541]	180° [217]	127.7° $[9\bar{1}\bar{1}\bar{1}]$	9	49	81	189
21*b*	27*b*	63*a*	180° [421]	180° [721]	23.0° $[01\bar{2}]$	9	49	81	189
27*a*	27*b*	81*a*	180° [511]	180° [217]	123.7° $[2\bar{1}\bar{1}1]$	9	81	81	243
27*a*	27*b*	81*b*	180° [511]	180° $[7\bar{1}2]$	38.9° $[1\bar{1}\bar{4}]$	9	81	81	243
27*b*	27*b*	81d	180° [721]	180° $[\bar{7}21]$	67.1° $[\bar{1}7\bar{7}]$	9	81	81	243

are sublattices of CSL_3. Indeed, as shown by Grimmer (1974*b*), there is a firm relationship between the CSL and DSC lattice. The DSC lattice is the reciprocal lattice of the CSL formed from the reciprocal lattices of the two crystals (in the case of the simple cubic structure the relationship is even simpler: the DSC lattice is the reciprocal lattice of the CSL). For $\alpha \neq 1$ junctions, Owusu-Boahen & King state that 'there is no simple relationship between the DSC lattices'. This is, actually, not completely correct. As shown in theorem 3, when $\alpha \neq 1$, the triple-junction CSL is a sublattice of all three grain-boundary CSLs. Fig. 1 gives a graphic illustration of this statement. The same can also be shown for less symmetrical configurations. Fig. 2 displays the same example, which was considered by Owusu-Boahen & King, *i.e.* a $\Sigma 9$–$\Sigma 33a$–$\Sigma 33b$ triple junction. In this junction, the triple-junction CSL, characterized by $\Sigma^{\rm TJ} = 99$, is a sublattice of all three grain-boundary CSLs. In such cases, the DSC lattice of the triple junction[5] contains DSC lattices of all three boundaries as sublattices (DSC lattices are not drawn in Fig. 2 not to over-complicate the figure).

It certainly remains a challenge for future research to show experimentally that $\alpha \neq 1$ junctions have different properties from other triple junctions.

6. Generalization for arbitrary crystal system

To extend the geometrical theory of triple junctions to non-cubic crystals, let us consider what in the analyses in §3 is general and what is specific only to the cubic crystal system. At first glance, theorem 1 does not contain any specifics of the crystal system and the Σ combination rule seems to be a general one. However, this is not so. The cubic crystal system is implied in equations (5). In the case of an arbitrary crystal lattice, the rotation matrix of a CSL misorientation can be represented as

$$R = \frac{1}{N}\{a_{ij}\}, \qquad (32)$$

where N is not necessarily equal to Σ. As the Σ theorem of Grimmer (1976) states, Σ is the least positive integer such that ΣR and ΣR^{-1} are integral matrices. Therefore, if

$$R = \frac{1}{N}\{a_{ij}\} \quad \text{and} \quad R^{-1} = \frac{1}{N'}\{a_{ij}\}, \qquad (33)$$

then Σ is the least common multiple of N and N'. In the cubic system, always $N = N' = \Sigma$, but this is not always true for an arbitrary crystal lattice. Thus, in a general case,

$$\Sigma = \zeta N, \qquad (34)$$

where ζ is a positive integer.

Now, let us analyze what will change in the derivation of the Σ combination rule. Instead of (10) and (11), we have

$$\frac{\zeta_1}{\Sigma_1}\{a_{ij}\}_1 \frac{\zeta_2}{\Sigma_2}\{a_{ij}\}_2 = \frac{\zeta_3}{\Sigma_3}\{a_{ij}\}_3^{-1}, \qquad (35)$$

$$\frac{\zeta_1}{\Sigma_1}\{a_{ij}\}_1 \frac{\zeta_2}{\Sigma_2}\{a_{ij}\}_2 = \frac{\zeta_1\zeta_2}{\Sigma_1\Sigma_2}\{b_{ij}\}. \qquad (36)$$

Matrix $\{b_{ij}\}$ is still calculated according to (12) and can have a common divisor α_{12}. Then, instead of (6), the Σ combination rule is

$$\Sigma_3 = \zeta_3\Sigma_1\Sigma_2/(\alpha_{12}\zeta_1\zeta_2). \qquad (37)$$

It follows from (37) that, for the α combination rule (see the corollary to theorem 1 in §3), instead of (13), one obtains

$$\alpha_{12}\alpha_{13}\alpha_{23} = \Sigma_1\Sigma_2\Sigma_3/(\zeta_1\zeta_2\zeta_3). \qquad (38)$$

To show how the Σ combination rule works, let us consider some numerical examples. Grimmer (1989) gives for a CSL with $\Sigma = 98$ in the rhombohedral lattice with the axial ratio $c/a = 2.711$ (which can be used to describe corundum-type oxides) the following rotation matrices

$$R_{\Sigma 98} = \frac{1}{14}\begin{pmatrix} 18 & 9 & 8 \\ -8 & 1 & -14 \\ -4 & 6 & 12 \end{pmatrix}, \quad R_{\Sigma 98}^{-1} = \frac{1}{98}\begin{pmatrix} 48 & -30 & -67 \\ 76 & 124 & 94 \\ -22 & -72 & 45 \end{pmatrix}. \qquad (39)$$

[5] By analogy with grain boundaries, the triple-junction DSC lattice can be defined as the coarsest lattice containing the three grain lattices as sublattices and it is conjectured that it is the reciprocal lattice of the CSL formed from the reciprocal lattices of the three crystals.

Consider $R_3 = R_1 R_2$, where $R_1 = R_2 = R_{\Sigma 98}$. In this case, $\zeta_1 = \zeta_2 = 7$ and

$$\{b_{ij}\} = \begin{pmatrix} 220 & 219 & 114 \\ -96 & -155 & -246 \\ -168 & 42 & 28 \end{pmatrix},$$
$$R_3^{-1} = \frac{1}{196}\begin{pmatrix} 220 & 219 & 114 \\ -96 & -155 & -246 \\ -168 & 42 & 28 \end{pmatrix}, \qquad (40)$$
$$R_3 = \frac{1}{1372}\begin{pmatrix} 214 & -48 & -1293 \\ 1572 & 904 & 1542 \\ -1074 & -1644 & -467 \end{pmatrix}.$$

One can see that $\alpha_{12} = 1$, $\zeta_3 = 7$ and $\Sigma_3 = 1372 = \Sigma_1 \Sigma_2 / 7$, which satisfies formula (37).

If we take $R_1 = R_2 = R_{\Sigma 98}^{-1}$, then $\zeta_1 = \zeta_2 = 1$ and

$$\{b_{ij}\} = 7\begin{pmatrix} 214 & -48 & -1293 \\ 1572 & 904 & 1542 \\ -1074 & -1644 & -467 \end{pmatrix},$$
$$R_3^{-1} = \frac{1}{1372}\begin{pmatrix} 214 & -48 & -1293 \\ 1572 & 904 & 1542 \\ -1074 & -1644 & -467 \end{pmatrix}, \qquad (41)$$
$$R_3 = \frac{1}{196}\begin{pmatrix} 220 & 219 & 114 \\ -96 & -155 & -246 \\ -168 & 42 & 28 \end{pmatrix}.$$

In this case, $\alpha_{12} = 7$, $\zeta_3 = 1$ and $\Sigma_3 = 1372 = \Sigma_1 \Sigma_2 / 7$, which again satisfies formula (37).

These examples show that theorem 2 is generally not true for an arbitrary crystal system. However, some particular solutions are still applicable. Let $\Sigma_1 = \zeta_1 N_1$, $\Sigma_2 = \zeta_2 N_2$ and

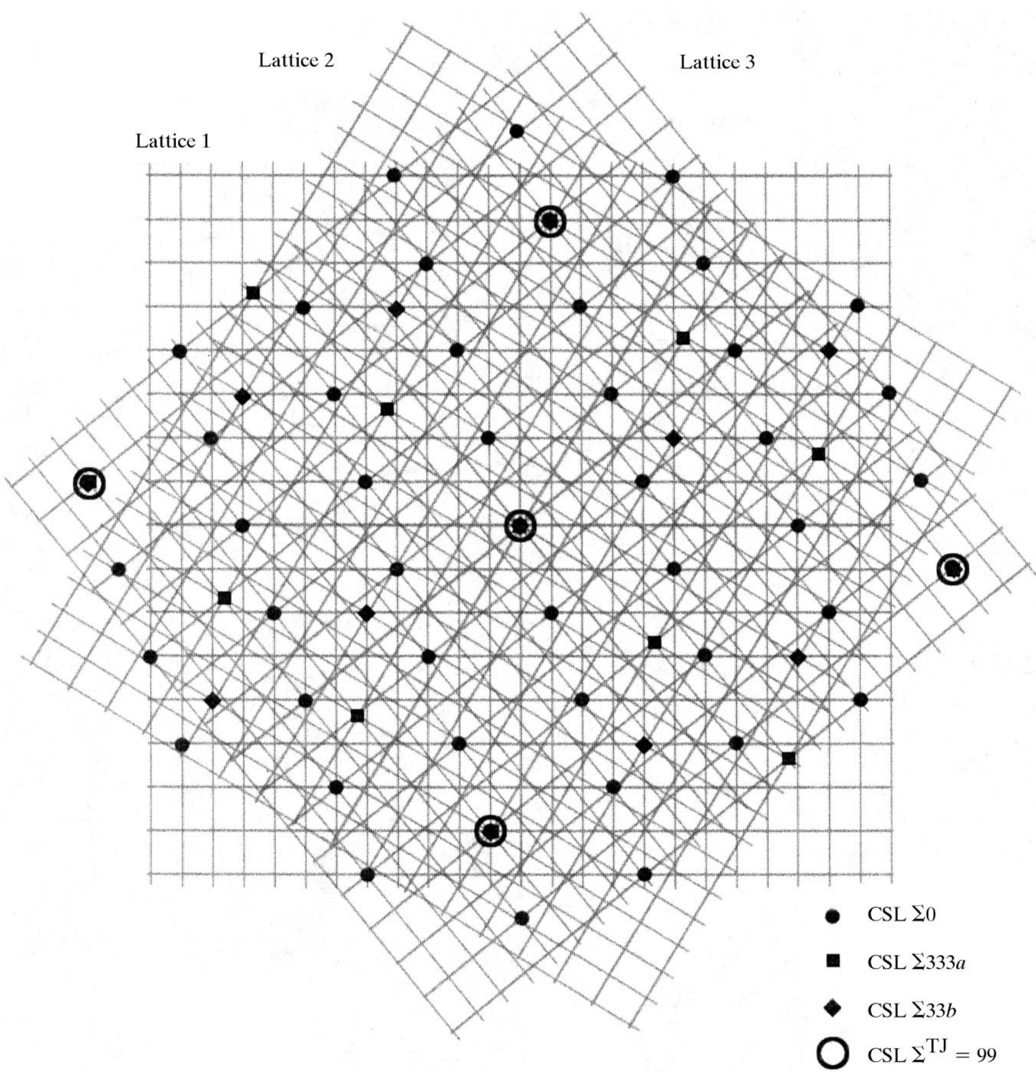

Figure 2
Superposition of three misoriented simple cubic lattices giving grain-boundary CSLs $\Sigma 9$, $\Sigma 33a$, $\Sigma 33b$ and triple-junction CSL with $\Sigma^{TJ} = 99$. The projection direction is [110].

Table 3
Combinations of CSL misorientations that cannot form triple junctions.

$\Sigma9$–$\Sigma21a$–$\Sigma21a$	$\Sigma21a$–$\Sigma27a$–$\Sigma63c$	$\Sigma27a$–$\Sigma27a$–$\Sigma81b$
$\Sigma9$–$\Sigma27a$–$\Sigma27a$	$\Sigma21a$–$\Sigma27b$–$\Sigma63b$	$\Sigma27a$–$\Sigma27a$–$\Sigma81d$
$\Sigma21a$–$\Sigma21a$–$\Sigma49b$	$\Sigma21b$–$\Sigma27a$–$\Sigma63b$	$\Sigma27a$–$\Sigma27b$–$\Sigma81c$
$\Sigma21a$–$\Sigma21a$–$\Sigma49c$	$\Sigma25a$–$\Sigma25a$–$\Sigma25a$	$\Sigma27a$–$\Sigma27b$–$\Sigma81d$
$\Sigma21a$–$\Sigma21b$–$\Sigma49a$	$\Sigma25a$–$\Sigma25a$–$\Sigma25b$	$\Sigma27b$–$\Sigma27b$–$\Sigma81b$
$\Sigma21a$–$\Sigma27a$–$\Sigma63a$	$\Sigma27a$–$\Sigma27a$–$\Sigma81a$	

$\Sigma_3 = \zeta_3 N_3$ [positive integers N have the meaning described by (32) and (34)]. It is easy to show that if $\alpha_{12} = 1$ then $\alpha_{13} = N_1^2$ and $\alpha_{23} = N_2^2$. If $N_1 = pq$, $N_2 = pr$ and $N_3 = qr$ [compare with (27)], then $\alpha_{12} = p^2$, $\alpha_{13} = q^2$, $\alpha_{23} = r^2$. However, it can be shown that in a general case of a non-cubic lattice $N_1 = pq$, $N_2 = pr$ and $N_3 = qrs$ (p, q, r, s are positive integers), and $\alpha_{12} = p^2/s$, $\alpha_{13} = q^2 s$, $\alpha_{23} = r^2 s$. This situation corresponds to the numerical example considered above and described by (41).

In the above examples, $(\Sigma_1\Sigma_2\Sigma_3)^{-1/2}$ is irrational, which demonstrates that formula (28) cannot be used for calculating $\Sigma^{\rm TJ}$. Apparently, it must be modified in the following way:

$$\begin{aligned}\Sigma^{\rm TJ} &= \zeta_1\zeta_2\zeta_3 pqrs/{\rm g.c.d.}(\zeta_1\zeta_2\zeta_3)\\ &= (\zeta_1\zeta_2\zeta_3\Sigma_1\Sigma_2\Sigma_3 s)^{1/2}/{\rm g.c.d.}(\zeta_1\zeta_2\zeta_3).\end{aligned} \quad (42)$$

This formula has been derived by considerations analogous to the analysis in theorem 3, but has not yet been carefully proven for the case when all three ζ's are different. Hence, in the general case it should still be considered a conjecture. The few examples of misorientations with $\zeta \neq 1$ that are known to the author all seem to satisfy formula (42). Another difference from the cubic system is that the case $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3 \neq 1$ is possible in some lattices. For example, consider Fig. 1(a) and assume that all the lattice planes parallel to this one have the same projection. This corresponds to the monoclinic lattice with $c/a = 7^{1/2}$ and $\beta = \arccos(-1/2 \times 7^{1/2}) \simeq 100.9^\circ$. The lattice in Fig. 1($a$) is then viewed along [010] and the b period can be arbitrary. In this case, $\Sigma^{\rm TJ} = \Sigma_1 = \Sigma_2 = \Sigma_3 = 3$.

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