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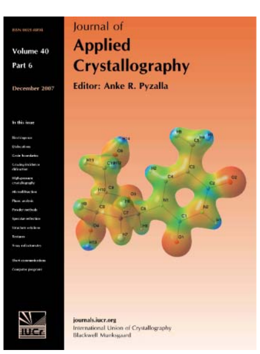

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Tilt and twist grain boundaries

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Grain boundaries are frequently classified into tilt, twist and mixed-type boundaries. However, the classification (into tilt and twist) is not a dichotomy; due to crystal symmetries, some boundaries may be concurrently tilt and twist boundaries. Formal conditions for a planar homophase boundary between crystals with $m3m$ symmetry to be a tilt as well as a twist boundary are determined, and a procedure for verification of whether a boundary has such dual character is given.

1. Introduction

In addition to grain boundary geometry, details of structure and bonding are needed for predicting boundary properties. However, assessment of geometry is the first step for all more in-depth analyses. Therefore, there is considerable interest in geometry-based classifications of boundaries. One such classification is the distinction between tilt, twist and mixed-type (or general) boundaries (see *e.g.* Sutton & Balluffi, 1995). Most grain boundary studies and experimental data concern tilt and twist boundaries in cubic materials.

Because of crystal symmetry, some pure twist boundaries can be also characterized as pure tilt boundaries. The best known example is the coherent twin boundary in face-centred cubic materials, which can be obtained by twisting a part of a crystal about the [111] direction by 60° or by tilting it about $[1\bar{1}0]$ by 70.53°.

In this paper, we address the problem of the formal conditions required for a planar homophase boundary between crystals with $m3m$ (O_h) symmetry to be simultaneously a tilt and a twist (or T and T) boundary. Similar conditions were briefly considered some time ago by Fortes (1973) but that approach was not complete.

2. Preliminaries

For specifying a boundary in a bicrystal, boundary parameters are needed. We will use the Cartesian coordinate systems defining the cubic lattices of crystals. Macroscopic boundary parameters can be given in the form of the 4 × 4 interface matrix

$$B = \begin{bmatrix} 0 & \mathbf{m}_2^T \\ \mathbf{m}_1 & M \end{bmatrix} \text{ with } \mathbf{m}_2 = -M^T\mathbf{m}_1, \qquad (1)$$

where M ($\neq$ identity matrix) is the 3 × 3 special orthogonal matrix of the misorientation between the coordinate systems of the first and second crystals, and $\mathbf{m}_1$ ($\mathbf{m}_2$) is the unit vector normal to the boundary plane given in the coordinate system of the first (second) crystal. Representations symmetrically equivalent to B have the form

$$\begin{bmatrix} 0 & (C_2\mathbf{m}_2)^T \\ C_1\mathbf{m}_1 & C_1MC_2^T \end{bmatrix} \text{ or } \begin{bmatrix} 0 & -(C_2\mathbf{m}_2)^T \\ -C_1\mathbf{m}_1 & C_1MC_2^T \end{bmatrix}, \qquad (2)$$

where C_i (i = 1, 2) are special orthogonal matrices of proper symmetry operations (Morawiec, 1998). A special orthogonal matrix can be expressed in a standard form as

$$\Psi_{ij}(\mathbf{n}, \alpha) = \delta_{ij}\cos\alpha + n_i n_j(1 - \cos\alpha) - \varepsilon_{ijk}n_k \sin\alpha, \qquad (3)$$

where $\mathbf{n}$ denotes a unit vector along the rotation axis and α denotes the rotation angle (see, for example, Morawiec, 2004). Explicit matrix components are used in equation (3) and summation over matrix indices which appear twice in a single term is assumed. The letter ε denotes the permutation symbol and δ is the Kronecker symbol.

For a tilt boundary, the rotation axis lies in the boundary plane. Thus, the vector $\mathbf{n}$ along the axis is perpendicular to the vectors $\mathbf{m}_i$, *i.e.* $\mathbf{m}_i \cdot \mathbf{n} = 0$ for i = 1, 2. We refer to a boundary as (properly) quasisymmetric if the crystallographic planes in the two crystals are symmetrically equivalent in the sense that $\mathbf{m}_2 = -C_0\mathbf{m}_1$, where C_0 is an orthogonal matrix representing a symmetry operation by (proper) rotation. For a twist boundary, the rotation axis is perpendicular to the boundary plane. Thus, the twist boundary can be parameterized in such a way that $\mathbf{m}_1 = -\mathbf{m}_2$, and these vectors are parallel to the rotation axis with $\mathbf{m}_1 = \mathbf{n} = -\mathbf{m}_2$, *i.e.* the interface matrix may have the form

$$B_{\text{twist}} = \begin{bmatrix} 0 & -\mathbf{n}^T \\ \mathbf{n} & \Psi(\mathbf{n}, \omega) \end{bmatrix}. \qquad (4)$$

B_{twist} is determined by misorientation parameters $\mathbf{n}$ and ω, with $-180° < \omega \leq 180°$.

3. T and T boundaries

There are two issues to be considered: first, what are the conditions for a given tilt boundary to be also a twist boundary, and second, what are the conditions for a given twist boundary to be a tilt boundary. We begin with the first one.

It is easy to see that for B' equivalent to $B_{\rm twist}$ the normals $\mathbf{m}_1 = C_1\mathbf{n}$ and $\mathbf{m}_2 = -C_2\mathbf{n}$ are related *via* $\mathbf{m}_2 = -C_2 C_1^T \mathbf{m}_1$, and the same occurs for $\mathbf{m}_1 = -C_1\mathbf{n}$ and $\mathbf{m}_2 = C_2\mathbf{n}$. Thus, every twist boundary has a proper quasisymmetric representation. A convenient way of recognizing the twist character of a boundary originates from the related statement: every proper quasisymmetric boundary is equivalent to a twist boundary. To show this, we assume that $\mathbf{m}_2 = -C_0\mathbf{m}_1$ for the boundary given by equation (1), and we consider its symmetrically equivalent representation obtained by application of $C_1 = C_0$,

$$\begin{bmatrix} 0 & \mathbf{m}_2^T \\ C_0\mathbf{m}_1 & C_0 M \end{bmatrix} = \begin{bmatrix} 0 & \mathbf{m}_2'^T \\ \mathbf{m}_1' & M' \end{bmatrix}. \qquad (5)$$

Based on equation (5) and $\mathbf{m}_2' = -M'^T\mathbf{m}_1'$, one has

$$\begin{aligned} \mathbf{m}_2' &= \mathbf{m}_2 = -C_0\mathbf{m}_1 = -\mathbf{m}_1', \\ M'^T\mathbf{m}_1' &= -\mathbf{m}_2' = \mathbf{m}_1' \quad \text{and} \\ M'\mathbf{m}_2' &= -\mathbf{m}_1' = \mathbf{m}_2', \end{aligned} \qquad (6)$$

i.e. $\mathbf{m}_2' = -\mathbf{m}_1'$ and both $\mathbf{m}_1'$ and $\mathbf{m}_2'$ are parallel to the rotation axis of M'. Thus, the representation in equation (5) satisfies the conditions for a twist boundary.

Now, we proceed to the question of which twist boundary is also a tilt boundary. Let B' be a symmetrically equivalent representation of $B_{\rm twist}$. If $C_1 = C_2$, the interface matrix B' also contains parameters with the rotation axis perpendicular to the boundary plane, *i.e.* it also explicitly represents a twist boundary[1]. This generally does not occur if C_1 and C_2 differ. The matrix B' will represent a tilt boundary if the normals $C_1\mathbf{n}$ and $C_2\mathbf{n}$ are perpendicular to the rotation axis of $C_1\Psi(\mathbf{n},\omega)C_2^T$. Since $C_1\Psi(\mathbf{n},\omega)C_2^T$ is a special orthogonal matrix, it can be expressed *via* Ψ,

$$C_1\Psi(\mathbf{n},\omega)C_2^T = \Psi(\mathbf{k},\beta), \qquad (7)$$

where $\mathbf{k}$ is a unit vector along the rotation axis and β is the rotation angle. For B' to be a tilt boundary, the relations $(C_i\mathbf{n})\cdot\mathbf{k} = 0$ must occur. The condition $(C_1\mathbf{n})\cdot\mathbf{k} = 0$ is equivalent to $\mathbf{n}\cdot\mathbf{k}' = 0$, where $\mathbf{k}' = C_1^T\mathbf{k}$. Let $C = C_2^T C_1$. Since $\Psi(\mathbf{k}',\beta) = C_1^T\Psi(\mathbf{k},\beta)C_1 = \Psi(\mathbf{n},\omega)C$, and for non-symmetric $\Psi(\mathbf{k}',\beta)$ the vector $\mathbf{k}'$ satisfies $k_i' \propto \varepsilon_{ijk}\Psi_{jk}(\mathbf{k}',\beta)$, the relation $\mathbf{n}\cdot\mathbf{k}' = 0$ leads to

$$\varepsilon_{ijk}\Psi_{jl}(\mathbf{n},\omega)C_{lk}n_i = 0. \qquad (8)$$

Using equation (3), one obtains

$$\varepsilon_{ijk}n_iC_{jk}\cos\omega - (C_{kk}\delta_{ij} - C_{ij})n_in_j\sin\omega = 0. \qquad (9)$$

If the matrix $\Psi(\mathbf{k}',\beta)$ is symmetric, one has $k_i'k_j' = [\delta_{ij} + \Psi(\mathbf{k}',\beta)_{ij}]/2$, and $\mathbf{n}\cdot(C_1^T\mathbf{k}) = n_ik_i' = 0$ can be replaced by $n_ik_i'k_j' = 0$ or

$$n_i + C_{ij}n_j = 0. \qquad (10)$$

One can proceed in the same way with the second condition $(C_2\mathbf{n})\cdot\mathbf{k} = 0$; it involves the matrix $C\Psi(\mathbf{n},\omega)$ instead of $\Psi(\mathbf{n},\omega)C$, and it leads to the same equations (9) and (10) depending on whether $C\Psi(\mathbf{n},\omega)$ is symmetric or not.

In order to obtain the parameters of twist boundaries which are T and T boundaries, we solve equations (9) and (10) to obtain the following solutions:

$$\omega = 180^\circ \text{ and arbitrary } \mathbf{n}, \qquad (\text{S1})$$

$$n_i = 0 \text{ for a given } i \text{ and arbitrary } \omega, \qquad (\text{S2})$$

$$n_i \pm n_j = 0 \text{ for } i \neq j \text{ and arbitrary } \omega, \qquad (\text{S3})$$

$$\tan(\omega/2) \pm n_i = 0 \text{ for a given } i, \qquad (\text{S4})$$

$$\tan(\omega/2) \pm n_1 \pm n_2 \pm n_3 = 0, \qquad (\text{S5})$$

where the 'zero' misorientation with $\omega = 0$ is excluded. Visualization of the last two cases (S4 and S5) in the angle–axis parameterization is complicated. More convenient for this are the Rodrigues parameters $r_i = n_i\tan(\omega/2)$ (Frank, 1988). With these, S1 has an awkward form

$$r_kr_k = \infty, \qquad (\text{S1})$$

but the remaining four are simple:

$$r_i = 0, \qquad (\text{S2})$$

$$r_i \pm r_j = 0, i \neq j, \qquad (\text{S3})$$

$$r_kr_k \pm r_i = 0, \qquad (\text{S4})$$

$$r_kr_k \pm r_1 \pm r_2 \pm r_3 = 0. \qquad (\text{S5})$$

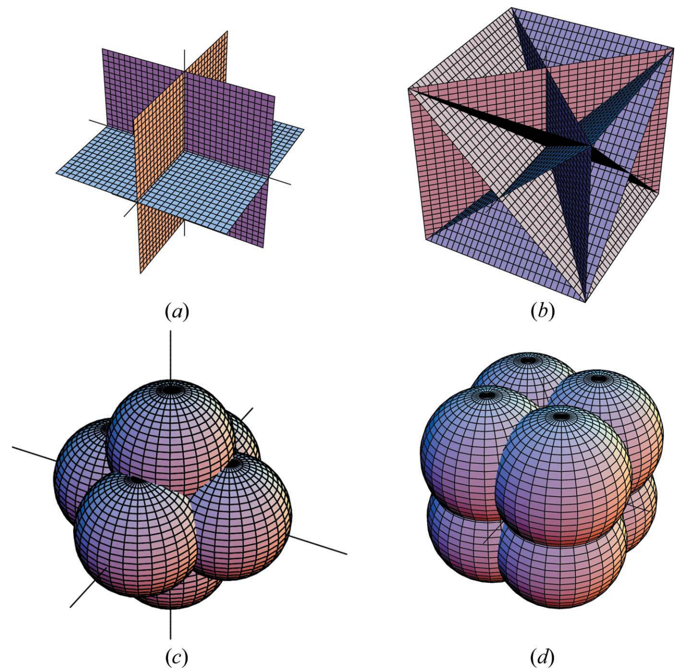

Figure 1
Schematic illustrations of Rodrigues 'vectors' given by solutions S2 (*a*), S3 (*b*), S4 (*c*) and S5 (*d*).

[1] An analogous statement applies to tilt boundaries: for an explicit representation of a tilt boundary with a rotation axis in the boundary plane, the symmetrically equivalent representation [equation (2)] based on $C_1 = C_2$ also satisfies the conditions for a tilt boundary.

These relations represent two-dimensional surfaces in the three-dimensional 'Rodrigues space'. Clearly, cases S2 and S3 are planes. Points satisfying relations S4 are located on six spheres of the same radius of 1/2 centred at (r_1, r_2, r_3) = $(\pm\frac{1}{2}, 0, 0)$, $(0, \pm\frac{1}{2}, 0)$ and $(0, 0, \pm\frac{1}{2})$. For case S5, these are eight spheres of radius $3^{1/2}/2$ centred at $(\pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$ (Fig. 1).

One may examine whether a given boundary has dual T and T character by completing the following steps. After determining the interface matrix, one needs to examine whether $\mathbf{m}_1$ and $\mathbf{m}_2$ are related by a proper symmetry operation. If this occurs, the considered case is a proper quasisymmetric boundary, and application of the symmetry operation to the initial interface matrix, as in equation (5), will lead to $B_{\rm twist}$ explicitly representing a twist boundary. The last step is to check whether $B_{\rm twist}$ satisfies any of the conditions S1–S5. If it does, the case under consideration is a T and T boundary. An example of this procedure is given in *Appendix A*.

For completeness, we recall related facts concerning symmetric tilt boundaries. A tilt boundary is referred to as symmetric if the boundary plane is a mirror plane between crystal structures. A mirror reflection with respect to a plane perpendicular to $\mathbf{m}$ is an improper rotation represented by the matrix $[\delta_{ij} - 2m_im_j]$. Since inversion is assumed to be a symmetry operation, the reflection is symmetrically equivalent to the proper rotation given by $-(\delta_{ij} - 2m_im_j) = \Psi_{ij}(\mathbf{m}, 180^\circ)$. This leads to the well known conclusion (*e.g.* Wolf & Lutsko, 1989) that every symmetric tilt boundary can also be seen as a 180° twist boundary. Conversely, a twist boundary is equivalent to a symmetric tilt boundary if it can be expressed as a 180° twist boundary. Moreover, the misorientation matrix $\Psi(\mathbf{k}, \omega)$ of the symmetric tilt boundary can be written as $\Psi(\mathbf{k}, \omega) = \Psi(\mathbf{m}, 180^\circ)C$, where $\mathbf{k}\cdot\mathbf{m} = 0$ and C is a special orthogonal matrix of a symmetry operation. Since $\Psi(\mathbf{k}, \omega)\mathbf{k} = \mathbf{k}$ and $\Psi(\mathbf{m}, 180^\circ)\mathbf{k} = -\mathbf{k}$, one has $C\mathbf{k} = -\mathbf{k}$. Therefore, C must be a half-turn, with the rotation axis $\mathbf{s}$ perpendicular to $\mathbf{k}$, *i.e.* $C = \Psi(\mathbf{s}, 180^\circ)$ and $\mathbf{s}\cdot\mathbf{k} = 0$. Since the only half-turns among the symmetry operations of $m3m$ are the rotations around ⟨100⟩ and ⟨110⟩, the rotation axis of a symmetric tilt boundary lies in one of the mirror planes {100} or {110} (see Sutton & Balluffi, 1995).

4. Final remarks

One may consider what would be the frequency of occurrence of T and T boundaries, or, assuming a certain tolerance, the fraction of such boundaries among randomly 'generated' boundaries. This is an aspect of the broader issue of frequencies of specific boundaries. The problem can be addressed numerically but the results will depend on an assumed measure in the boundary space.

The discussion of the structure or dislocation content of T and T boundaries is beyond the scope of this work. However, it is worth mentioning that low-Σ coincident lattice (CSL) misorientations satisfy the conditions for being T and T. The lowest Σ which cannot correspond to a T and T boundary is Σ39 ([123], 50.13°). Some CSL misorientations comply with multiple conditions (*e.g.* Σ3 satisfies all conditions S1–S5). Most low-Σ CSL misorientations fit some of conditions S1, S2 and S3; the first one fulfilling conditions S4 and S5 but no other is Σ63 ([123], 56.25°). A twist boundary which has integer Miller indices and which satisfies relations S1, S4 or S5 is a CSL boundary.

Complete characterization of the geometry of a boundary is not always simple. The conditions for T and T listed in this paper may make the task somewhat easier. Only the case of $m3m$ crystal symmetry has been analysed here, but a similar approach can be applied to other symmetries. For non-cubic lattices, the manipulations will be less convenient but the general principles will be the same. Some differences will appear if the crystals have no inversion symmetry.

APPENDIX *A*

An example is given of the procedure for checking whether a given boundary is T and T. Let us take the boundary with the planes (245) and $(\overline{2}\overline{5}4)$, with the misorientation given by rotation axis [11 9 1] and rotation angle arccos(−11/18). The boundary is represented by the matrix

$$B = \begin{bmatrix} 0 & -2a & -5a & 4a \\ 2a & 22b & 46b & 37b \\ 4a & 53b & 2b & -34b \\ 5a & -26b & 43b & -38b \end{bmatrix},$$

where $a = 5^{1/2}/15$ and $b = 1/63$. The vectors normal to the boundary plane are related by the symmetry operation C_0 = $\Psi([1,0,0]^T, 270^\circ) = [\delta_{1i}\delta_{1j} + \varepsilon_{1ij}]$; one has $[\overline{2}\overline{5}4]^T = -C_0[245]^T$. Thus, B corresponds to a proper quasisymmetric boundary. Application of the symmetry operation $C_1 = C_0$ to B gives the representation

$$B_{\rm twist} = \begin{bmatrix} 0 & -2a & -5a & 4a \\ 2a & 22b & 46b & 37b \\ 5a & -26b & 43b & -38b \\ -4a & -53b & -2b & 34b \end{bmatrix},$$

with the plane Miller indices $(25\overline{4})$ and $(\overline{2}\overline{5}4)$ and rotation axis $[25\overline{4}]$ perpendicular to the boundary plane, *i.e.* with the explicit characteristics of a twist boundary. For the above $B_{\rm twist}$, one has $n = (5^{1/2}/15)[2, 5, -4]^T$ and $\tan(\omega/2) = 5^{1/2}/3$, and these parameters satisfy S4. Thus, the boundary being considered has dual T and T character. Indeed, the symmetry operation $C_2 = \Psi([0,1,0]^T, 90^\circ) = [\delta_{2i}\delta_{2j} - \varepsilon_{2ij}]$ leads to

$$B' = \begin{bmatrix} 0 & 4a & -5a & 2a \\ 2a & 37b & 46b & -22b \\ 5a & -38b & 43b & 26b \\ -4a & 34b & -2b & 53b \end{bmatrix},$$

with the planes $(25\overline{4})$ and $(4\overline{5}2)$ and rotation axis $[\overline{1}\overline{2}\overline{3}]$ in the boundary plane, *i.e.* B' explicitly represents a tilt boundary.

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