Constructing Dislocation Models of Low-Angle Grain Boundaries

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Introduction

Frank's formulas [1, 2] provide a sufficient mathematical condition for a planar arrangement of dislocations to form a grain boundary (*i.e.,* have no long range stresses). Unfortunately, it does not actually provide a prescription for constructing a dislocation model of grain boundary defined in terms of its macroscopic parameters (*e.g.,* misorientation, inclination, etc.). While subsequent researchers have reformulated Frank's formulas in many ways that bridge the gap between the macro- and meso-scopic descriptions of grain boundaries [3], a set of explicit rules for converting between macro- and meso-scopic descriptions of grain boundaries appears to be lacking from the literature. Moreover, there seems to be some general confusion about what parameters are required to provide a complete description of a grain boundary at the macroscopic level. These notes attempts to shed light on both of these issues.

Macroscopic Descriptions of Grain Boundaries

At the macroscopic level, it is often thought that five parameters are sufficient to uniquely define a three-dimensional grain boundary: the misorientation (3 parameters) and the inclination of the plane (2 parameters) between the neighboring grains. Unfortunately, even if we ignore the three degrees of freedom associated with the translation of the grains relative to each other[1], this description is incomplete. What is missing from the five parameter description of a grain boundary is the orientation of one of the grains, which requires three *additional* parameters[2]. The key (but subtle) point that is often overlooked, is that the misorientation only gives the orientations of the grains *relative* to each other. We need to specify the orientation of one of the grains in order to uniquely describe the grain boundary. Thus, a complete description of a general three-dimensional grain boundary requires a total of eight parameters[3].

The common approach of specifying only the misorientation of the neighboring grains and the inclination of the grain boundary is sufficient only when we *implicitly* assume that both the misorientation and inclination are specified in a coordinate system attached to one of the grains. In effect, the orientation of one of the grains has been specified so that a five parameter description of the grain boundary is acceptable. This approach

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[1]Ignoring these degrees of freedom is usually acceptable because translations by less than one unit cell are negligible at macro- and meso-scopic length scales.

[2]In two-dimensions, only one additional parameter is required to specify the orientation of one of the grains.

[3]A general two-dimensional grain boundary requires a total of three parameters.

breaks down if one wishes to describe the grain boundary in a coordinate system that is independent of either of the neighboring grains (*e.g.,* using a simulation coordinate system).

Tilt Grain Boundaries

Tilt grain boundaries are defined by the condition that the misorientation axis lies within the grain boundary. This condition places one constraint on the misorientation axis, so the number of parameters required to describe a tilt grain boundary is reduced from eight to seven. Symmetric tilt grain boundaries requires even fewer parameters to define because the plane of the grain boundary is further constrained to be a mirror planes for one of the grains. This constraint removes the two degrees of freedom associated with the direction of the grain boundary normal, so symmetric tilt grain boundaries require only five parameters to be uniquely defined.

Twist Grain Boundaries

Pure twist grain boundaries are defined by the condition that the misorientation axis is perpendicular to the grain boundary plane. This constraint eliminates the degrees of freedom for the misorientation axis (or equivalently the orientation of the grain boundary plane). Thus, twist grain boundaries are uniquely defined by six parameters.

Dislocation Models of Low-Angle Grain Boundaries

At the mesoscopic level, low-angle grain boundaries can be constructed from arrays of straight dislocations. These dislocation models of grain boundaries, which were originally developed by Frank, Read, and Shockley [2, 3], are useful starting points for studying the structure and properties of low-angle grain boundaries. While equilibrium grain boundary structures are not always composed solely of straight dislocation lines, straight line dislocation models can always be relaxed to obtain equilibrium grain boundary structures. In this section, we give explicit procedures for constructing dislocation models of several common grain boundaries.

Tilt Grain Boundaries

One Set of Dislocations

When only a single set of dislocations is used to form a grain boundary, the result is a symmetric tilt grain boundary. The dislocation model is defined by specifying the Burgers vector, $\boldsymbol{b}$, the direction of the dislocation line, $\hat{\boldsymbol{\xi}}$, and the interdislocation spacing, D. These mesoscopic parameters satisfy the following conditions:

- the Burgers vector, $\boldsymbol{b}$, is perpendicular to the grain boundary plane (*i.e.,* $\boldsymbol{b} \parallel \hat{\boldsymbol{\nu}}$);
- $\hat{\boldsymbol{\xi}}$ is parallel to the misorientation axis, $\hat{\boldsymbol{u}}$; and
- D satisfies

$$D = \frac{|\boldsymbol{b}|}{2\sin(\theta/2)}. \tag{1}$$

These conditions imply that all the dislocations in the array are pure edge dislocations because the Burgers vector is perpendicular to the dislocation line direction. Notice that the number of mesoscopic parameters required to specify a symmetric tilt grain boundary using only one set of dislocations is five, which is the same as the number of parameters required for macroscopic description: 3 for $\boldsymbol{b}$, 1 for $\hat{\boldsymbol{\xi}}$, and 1 for D. Note that there is only one degree of freedom for $\hat{\boldsymbol{\xi}}$ because it is constrained to lie in the grain boundary plane.

To construct a symmetric tilt grain boundary formed from only a single set of dislocations, we first choose the Burgers vector, $\boldsymbol{b}$ and the direction of the dislocation lines, $\hat{\boldsymbol{\xi}}$ so that $\boldsymbol{b} \cdot \hat{\boldsymbol{\xi}} = 0$. Once $\boldsymbol{b}$ and $\hat{\boldsymbol{\xi}}$ are chosen, the grain boundary normal and misorientation axis are set: $\hat{\boldsymbol{\nu}} = \boldsymbol{b}/|\boldsymbol{b}|$ and $\hat{\boldsymbol{u}} = \hat{\boldsymbol{\xi}}$. Finally, we choose the misorientation angle, θ, between the neighboring grains and compute D using (1).

Two Sets of Dislocations

Dislocation models of general tilt grain boundaries require the use of at least two sets of dislocations. For each set of dislocations, we specify the Burgers vector, the direction of the dislocation line, and the interdislocation spacing. Dislocation models composed of two sets of dislocations are defined by $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\hat{\boldsymbol{\xi}}_1$, $\hat{\boldsymbol{\xi}}_2$, D_1, and D_2. For tilt boundaries, these mesoscopic parameters satisfy the following conditions:

- $(\boldsymbol{b}_1 \times \boldsymbol{b}_2)$ lies in the plane of the grain boundary;
- $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$ are both parallel to the misorientation axis, $\hat{\boldsymbol{u}}$, which lies in the plane of the grain boundary; and
- D_1 and D_2 satisfy

$$\frac{1}{2D_1 \sin(\theta/2)} = \frac{\boldsymbol{b}_2 \cdot (\hat{\boldsymbol{u}} \times \hat{\boldsymbol{\nu}})}{\hat{\boldsymbol{u}} \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_1)} \tag{2}$$

$$\frac{1}{2D_2 \sin(\theta/2)} = \frac{-\boldsymbol{b}_1 \cdot (\hat{\boldsymbol{u}} \times \hat{\boldsymbol{\nu}})}{\hat{\boldsymbol{u}} \cdot (\boldsymbol{b}_2 \times \boldsymbol{b}_1)} \tag{3}$$

These conditions reduce the degrees of freedom available to the mesoscopic dislocation parameters by one, three, and one, respectively. Therefore, the total number of mesoscopic parameters required to describe a tilt grain boundary is seven, which agrees with the the number of parameters needed to a general tilt grain boundary at the macroscopic level. Notice that to avoid trivial grain boundaries where $\theta = 0$ or $D_i = \infty$, (2) and (3) impose certain relationships between $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\hat{\boldsymbol{u}}_1$, $\hat{\boldsymbol{u}}_2$, $\hat{\boldsymbol{\nu}}_1$, and $\hat{\boldsymbol{\nu}}_2$:

- $(\boldsymbol{b}_1 \times \boldsymbol{b}_2)$ must *not* be orthogonal to $\hat{\boldsymbol{u}}$; and
- $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ must *not* be orthogonal to $(\hat{\boldsymbol{u}} \times \hat{\boldsymbol{\nu}})$.

These constraints do not reduce the number of parameters required to define the dislocation model of the grain boundary.

To construct general tilt grain boundaries using two sets of dislocations, we first choose the two Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. We are then free to choose the normal vector to the grain boundary plane, $\hat{\boldsymbol{\nu}}$, so that it satisfies $(\boldsymbol{b}_1 \times \boldsymbol{b}_2) \cdot \hat{\boldsymbol{\nu}} = 0$. Once we have $\hat{\boldsymbol{\nu}}$, we choose $\hat{\boldsymbol{u}} = \hat{\boldsymbol{\xi}}_1 = \hat{\boldsymbol{\xi}}_2$ such that $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{\nu}} = 0$ and $(\boldsymbol{b}_1 \times \boldsymbol{b}_2) \cdot \hat{\boldsymbol{u}} \neq 0$. Finally, we choose the misorientation angle, θ, and compute D_1 and D_2 using (2) and (3).

Symmetric Tilt Boundaries The mirror symmetry (at the continuum level) of two dislocation models of symmetric tilt boundaries require that the plane of the grain boundary and the misorientation axis satisfy special relationships to the Burgers vectors:

$$\hat{\boldsymbol{\nu}} = \frac{1}{|\boldsymbol{b}_1|\sqrt{2(1+\cos\alpha)}}\boldsymbol{b}_1 + \frac{1}{|\boldsymbol{b}_2|\sqrt{2(1+\cos\alpha)}}\boldsymbol{b}_2, \tag{4}$$

$$\hat{\boldsymbol{u}} = \frac{\boldsymbol{b}_1 \times \boldsymbol{b}_2}{|\boldsymbol{b}_1 \times \boldsymbol{b}_2|} \tag{5}$$

where α is the angle between $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. Using the expression in (4) for $\hat{\boldsymbol{\nu}}$, (2) and (3) simplify to

$$D_1 = -\frac{|\boldsymbol{b}_1|\sqrt{2(1+\cos\alpha)}}{2\sin(\theta/2)}\ ,\ D_2 = -\frac{|\boldsymbol{b}_2|\sqrt{2(1+\cos\alpha)}}{2\sin(\theta/2)} \tag{6}$$

Note that these expressions also impose a constraint on the interdislocation spacings:

$$|\boldsymbol{b}_1|/D_1 = |\boldsymbol{b}_2|/D_2. \tag{7}$$

A detailed derivation of these relations is given in Appendix A.

To construct a two dislocation model of a symmetric tilt grain boundary, we first choose the two Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. We then compute the normal to the grain boundary plane using (4). Next, we compute the misorientation axis (and line directions) using (5). Finally, we choose the misorientation angle, θ, and compute D_1 and D_2 using (6). Note that D_1 and D_2 computed in this manner automatically satisfy (7). As expected, the specification of a symmetric tilt boundary has two fewer degrees of freedom than the specification for a general tilt boundary.

Twist Grain Boundaries

Dislocation models of pure twist grain boundaries require the use of at least two sets of dislocations. For two dislocation models, twist boundaries are characterized by the following conditions:

- both $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ lie in the plane of the grain boundary;
- both $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$ lie in the plane of the grain boundary;
- the misorientation axis, $\hat{\boldsymbol{u}}$, is parallel to the grain boundary normal, $\hat{\boldsymbol{\nu}}$; and
- D_1 and D_2 satisfy

$$\frac{1}{2D_1|\sin(\theta/2)|} = \frac{|\boldsymbol{b}_2|}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{8}$$

$$\frac{1}{2D_2|\sin(\theta/2)|} = \frac{|\boldsymbol{b}_1|}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{9}$$

- $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$ satisfy

$$\hat{\boldsymbol{\xi}}_1 = -\mathrm{sgn}(\theta)\left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_2}{|\boldsymbol{b}_2|}\right) \tag{10}$$

$$\hat{\boldsymbol{\xi}}_2 = \mathrm{sgn}(\theta)\left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_1}{|\boldsymbol{b}_1|}\right). \tag{11}$$

A detailed derivation of these relations is given in Appendix B.

It is important to point out that these conditions reduce the total number of parameters for the dislocation model to five, which is *less* than the number of parameters required for the macroscopic description of a general twist grain boundary. The reason for this discrepancy is that two dislocation models of twist boundaries are *unable* to represent the most general twist boundaries – they boundaries are only able to represent twist boundaries where the Burgers vectors for the dislocations *all* lie in the plane of the grain boundary. In general, twist boundaries need not satisfy this constraint.

Using these conditions, we construct two dislocation models of twist boundaries by first choosing two Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. We then compute the normal to the grain boundary plane and the misorientation axis as $\hat{\boldsymbol{\nu}} = \hat{\boldsymbol{u}} = \boldsymbol{b}_1 \times \boldsymbol{b}_2$. Next, we choose the misorientation angle, θ, and compute D_1 and D_2 using (8) and (9). Finally, we compute the directions of the dislocation lines using (10) and (11).

Arbitrary Grain Boundaries

Dislocation models of arbitrary grain boundaries require the use of at least two sets of dislocations. For two dislocation models, arbitrary grain boundaries are characterized by the following conditions:

- the misorientation axis, $\hat{\boldsymbol{u}}$, is parallel to $(\boldsymbol{b}_1 \times \boldsymbol{b}_2)$;
- both $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$ lie in the plane of the grain boundary;
- D_1 and D_2 satisfy

$$\frac{1}{2D_1|\sin(\theta/2)|} = \frac{|\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)|}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{12}$$

$$\frac{1}{2D_2|\sin(\theta/2)|} = \frac{|\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)|}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{13}$$

- $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$ satisfy

$$\hat{\boldsymbol{\xi}}_1 = -\mathrm{sgn}(\theta)\left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)}{|\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)|}\right) \tag{14}$$

$$\hat{\boldsymbol{\xi}}_2 = \mathrm{sgn}(\theta)\left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)}{|\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}}(\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)|}\right). \tag{15}$$

A detailed derivation of these relations is given in Appendix C.

The conditions for two dislocation models of arbitrary grain boundaries leads to a mesoscopic grain boundary model with only seven free parameters, which is *less* than the number of parameters required for the macroscopic description of an arbitrary grain boundary. As with two dislocation models of twist boundaries, the reason for this discrepancy is that two dislocation models of arbitrary grain boundaries are only able to represent the a restricted subclass of arbitrary grain boundaries. Three dislocation models are necessary in order to represent the full range of grain boundaries.

Using these conditions, we construct two dislocation models of arbitrary grain boundaries by first choosing two Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$. We then arbitrarily choose a grain boundary normal, $\hat{\boldsymbol{\nu}}$, and calculate the misorientation axis using $\hat{\boldsymbol{u}} = \boldsymbol{b}_1 \times \boldsymbol{b}_2$. Next, we choose the misorientation angle, θ, and compute D_1 and D_2 using (12) and (13). Finally, we compute the directions of the dislocation lines using (14) and (15).

A Derivations for Two Dislocation Model of Symmetric Tilt Grain Boundaries

The normal to the grain boundary plane, $\hat{\boldsymbol{\nu}}$, and the misorientation axis, $\hat{\boldsymbol{u}}$, are calculated in this appendix. We begin by defining $\hat{\boldsymbol{\nu}}$ as a weighted sum of the Burgers vectors:

$$\hat{\boldsymbol{\nu}} = w_1 \boldsymbol{b}_1 + w_2 \boldsymbol{b}_2, \tag{16}$$

with $w_1^2 + w_2^2 = 1$. Note that this choice of $\hat{\boldsymbol{\nu}}$ guarantees $(\boldsymbol{b}_1 \times \boldsymbol{b}_2)$ lies in the grain boundary plane because $\hat{\boldsymbol{\nu}} \cdot (\boldsymbol{b}_1 \times \boldsymbol{b}_2) = 0$. By geometric reasoning, in order for the tilt grain boundary to be symmetric, we need the projections of the Burgers vectors onto $\hat{\boldsymbol{\nu}}$ and the directions orthogonal to $\hat{\boldsymbol{\nu}}$ to satisfy

$$\frac{\boldsymbol{b}_1}{D_1} \cdot \hat{\boldsymbol{\nu}} = \frac{\boldsymbol{b}_2}{D_2} \cdot \hat{\boldsymbol{\nu}} \tag{17}$$

$$\frac{\boldsymbol{b}_1}{D_1} \times \hat{\boldsymbol{\nu}} = -\frac{\boldsymbol{b}_2}{D_2} \times \hat{\boldsymbol{\nu}}. \tag{18}$$

Substituting (16) into these equations, we find that

$$\frac{w_1}{D_1}|\boldsymbol{b}_1|^2 + \frac{w_2}{D_1}(\boldsymbol{b}_1 \cdot \boldsymbol{b}_2) = \frac{w_1}{D_2}(\boldsymbol{b}_1 \cdot \boldsymbol{b}_2) + \frac{w_2}{D_2}|\boldsymbol{b}_2|^2 \tag{19}$$

$$\frac{w_2}{D_1}(\boldsymbol{b}_1 \times \boldsymbol{b}_2) = -\frac{w_1}{D_2}(\boldsymbol{b}_2 \times \boldsymbol{b}_1). \tag{20}$$

Rearranging these equations under the assumption that $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are not collinear yields the simple relations $|\boldsymbol{b}_1|/D_1 = |\boldsymbol{b}_2|/D_2$ and $w_1|\boldsymbol{b}_1| = w_2|\boldsymbol{b}_2|$. Recalling that $\hat{\boldsymbol{\nu}}$ should be a unit vector, we find that

$$w_1 = \frac{1}{|\boldsymbol{b}_1|\sqrt{2\,(1+\cos\alpha)}} \tag{21}$$

$$w_2 = \frac{1}{|\boldsymbol{b}_2|\sqrt{2\,(1+\cos\alpha)}}, \tag{22}$$

where α is the angle between $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$.

Assuming that $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are linearly independent, (16) and the fact that the misorientation axis lies in the grain boundary plane for tilt boundaries imply that u must be perpendicular to both Burgers vectors. Therefore, we may set the misorientation axis using

$$\hat{\boldsymbol{u}} = \frac{\boldsymbol{b}_1 \times \boldsymbol{b}_2}{|\boldsymbol{b}_1 \times \boldsymbol{b}_2|} \tag{23}$$

B Derivations for Two Dislocation Model of Twist Grain Boundaries

For two dislocation models of twist grain boundaries, Frank's rules imply that [1]

$$\frac{1}{2D_1 \sin(\theta/2)}(\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_1) = \frac{\boldsymbol{b}_2}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{24}$$

$$\frac{1}{2D_2 \sin(\theta/2)}(\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_2) = \frac{-\boldsymbol{b}_1}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|}. \tag{25}$$

To derive the equations for D_1 and D_2, we take the modulus of these two equations to arrive at (8) and (9). Substituting these expressions back into (24) and (25) and recognizing that $\sin(\theta/2)$ and θ have the same sign, we find that

$$\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_1 = \mathrm{sgn}(\theta) \left(\frac{\boldsymbol{b}_2}{|\boldsymbol{b}_2|} \right) \tag{26}$$

$$\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_2 = -\mathrm{sgn}(\theta) \left(\frac{\boldsymbol{b}_1}{|\boldsymbol{b}_1|} \right). \tag{27}$$

To solve for $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$, we take the cross product of these equations by $\hat{\boldsymbol{\nu}}$ and use the fact that the dislocation lines lie in the grain boundary plane (*i.e.,* $\hat{\boldsymbol{\xi}}_i \cdot \hat{\boldsymbol{\nu}} = 0$):

$$\hat{\boldsymbol{\xi}}_1 = -\mathrm{sgn}(\theta) \left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_2}{|\boldsymbol{b}_2|} \right) \tag{28}$$

$$\hat{\boldsymbol{\xi}}_2 = \mathrm{sgn}(\theta) \left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_1}{|\boldsymbol{b}_1|} \right). \tag{29}$$

C Derivations for Two Dislocation Model of Arbitrary Grain Boundaries

For two dislocation models of arbitrary grain boundaries, Frank's rules imply that [1]

$$\frac{1}{2D_1 \sin(\theta/2)} (\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_1) = \frac{\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|} \tag{30}$$

$$\frac{1}{2D_2 \sin(\theta/2)} (\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_2) = \frac{-\boldsymbol{b}_1 + \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)}{|\boldsymbol{b}_2 \times \boldsymbol{b}_1|}. \tag{31}$$

To derive the equations for D_1 and D_2, we take the modulus of these two equations to arrive at (12) and (13). Substituting these expressions back into (30) and (31) and recognizing that $\sin(\theta/2)$ and θ have the same sign, we find that

$$\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_1 = \mathrm{sgn}(\theta) \left(\frac{\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)}{|\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)|} \right) \tag{32}$$

$$\hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{\xi}}_2 = -\mathrm{sgn}(\theta) \left(\frac{\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)}{|\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)|} \right). \tag{33}$$

To solve for $\hat{\boldsymbol{\xi}}_1$ and $\hat{\boldsymbol{\xi}}_2$, we take the cross product of these equations by $\hat{\boldsymbol{\nu}}$ and use the fact that the dislocation lines lie in the grain boundary plane (*i.e.,* $\hat{\boldsymbol{\xi}}_i \cdot \hat{\boldsymbol{\nu}} = 0$):

$$\hat{\boldsymbol{\xi}}_1 = -\mathrm{sgn}(\theta) \left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)}{|\boldsymbol{b}_2 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_2)|} \right) \tag{34}$$

$$\hat{\boldsymbol{\xi}}_2 = \mathrm{sgn}(\theta) \left(\hat{\boldsymbol{\nu}} \times \frac{\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)}{|\boldsymbol{b}_1 - \hat{\boldsymbol{\nu}} (\hat{\boldsymbol{\nu}} \cdot \boldsymbol{b}_1)|} \right). \tag{35}$$

Transformation to Simulation Coordinates

When simulating dislocation models of grain boundaries, it is convenient to use a coordinate system that differs from the crystal coordinate system. The transformation from the crystal to the simulation coordinate is straightforward to compute. First, choose an orthogonal basis vectors for the simulation frame, $\{\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \hat{\boldsymbol{e}}_3\}$, in the crystal coordinate system. Then the transformation matrix from the simulation coordinate to the crystal coordinate system is given by

$$T = [\hat{\boldsymbol{e}}_1 | \hat{\boldsymbol{e}}_2 | \hat{\boldsymbol{e}}_3] \,. \tag{36}$$

Because this is an orthogonal transformation, the inverse transformation from the crystal to the simulation coordinate system is simply the transpose of T.

For tilt boundaries, it is natural to choose the following simulation frame:

$$\hat{\boldsymbol{e}}_1 = \hat{\boldsymbol{\nu}} \ , \ \hat{\boldsymbol{e}}_2 = \hat{\boldsymbol{u}} \ , \ \hat{\boldsymbol{e}}_3 = \hat{\boldsymbol{\nu}} \times \hat{\boldsymbol{u}}. \tag{37}$$

Note that the third coordinate axis for the simulation is chosen to ensure a right-handed, orthogonal coordinate system for the simulation frame.

For twist boundaries, it is natural to choose the $\hat{\boldsymbol{e}}_1 = \hat{\boldsymbol{\nu}}$. The second coordinate axis for the simulation can be chosen arbitrarily such that $\hat{\boldsymbol{e}}_2 \cdot \hat{\boldsymbol{e}}_1 = 0$. The third coordinate axis can be computed to ensure a right-handed, orthogonal coordinate system for the simulation frame: $\hat{\boldsymbol{e}}_3 = \hat{\boldsymbol{e}}_1 \times \hat{\boldsymbol{e}}_2$.

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