J Mater Sci (2006) 41:7669–7674
DOI 10.1007/s10853-006-0592-8

Metrics, measures, and parametrizations for grain boundaries: a dialog

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Received: 3 April 2006 / Accepted: 19 June 2006 / Published online: 24 October 2006

Abstract Analysis of experimental data on grain boundaries (GBs) can involve putting data into angle ''bins.'' An example is Brandon's classification: if rotation angle and axis are each within $15^\circ/\sqrt{\Sigma}$ of a perfect coincidence site lattice (CSL) with density $1/\Sigma$, the GBs can also be considered to be in that CSL relationship, and not if otherwise. Other examples of binning are studies of GB distributions in the full 5D angle space. To determine the size of a bin (necessary for densities, gradients, etc.) one must find a useful way, respecting symmetry, of determining metrics and measures on the full 5-dimensional space of both misorientation and interface normal. For a pair of low-angle GBs, the issue of metric is complicated by the fact that both their rotation axes and their GB normals can stay far apart as their rotation angles approach zero. We address all these issues as a dialog, and provide a framework for choosing metrics.

1. Old metallurgist: One of David Brandon's important contributions is a widely used, easy-to-apply, classification of grain boundaries (GBs) into special or general GBs for cubic crystals. He suggests that a GB is ''special'' if the orientation relationship of abutting crystals is ''close enough'' to a coincidence site lattice (CSL) relation, where ''close enough'' means if two of the angles characterizing their misorientation are less than $15/\sqrt{\Sigma}$ from those of a CSL. All others are general GBs. What do you make of this measure of angular differences between grain boundaries?

Young mathematician: Ah, you are referring to the following excerpt from Brandon's *The Structure of High Angle Grain Boundaries* [1]: ''The maximum permissible deviation for coincidence may reasonably be assumed to be given by ... $\theta_0\Sigma^{-1/2}$... where $\theta_0 \simeq 15^\circ \ldots$ Each coincidence lattice covers a range of $4\pi(1 - \cos(\theta_0/\Sigma^{1/2}))$ in axis of misorientation and a range $\theta_0/\Sigma^{1/2}$ in angular deviation.'' To me, on closer examination, it actually gives rise to a very interesting concept of closeness, which I'll call d_B, a ''Brandon-distance'' which is not symmetric, not finite, and doesn't obey the triangle inequality, all of them conditions that must be met for the mathematical definition of a distance. Suppose a CSL with fraction $1/\Sigma_0$ of common sites is produced when a cubic lattice is rotated about $\mathbf{u}_1$ by θ_1, where $\mathbf{u}_1$ is a unit vector and θ_1 an angle in $(0, \pi)$. Suppose $(\mathbf{u}, \theta)$ is any other axis–angle pair. Define

$$d_B((\mathbf{u},\theta),(\mathbf{u}_1,\theta_1)) = \Sigma_0^{1/2}\max\{|\theta-\theta_1|, \arccos(\mathbf{u}\cdot\mathbf{u}_1)\}.$$

We can now rewrite Brandon's criterion for the rotation Θ, specified by $(\mathbf{u}, \theta)$, being close to the rotation Θ_1, specified by $(\mathbf{u}_1, \theta_1)$, as

$$d_B((\mathbf{u},\theta),(\mathbf{u}_1,\theta_1)) < \pi/12.$$

(Observe that the $\Sigma^{1/2}$ is in the definition of d_B rather than as a factor dividing the $\pi/12$.) Actually, Brandon is

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somewhat unclear here; he said that the maximum deviation should be $\pi/(12\Sigma^{1/2})$ and applied that statement correctly for the axis, but then said that the range of the angle of rotation should be that quantity rather than twice that quantity (allowing the angle to be more or less than that for perfect coincidence). I'm going with the word ''deviation.'' Also, he effectively limits his axes to the upper hemisphere (in fact, to a particular spherical triangle) and allows the angle of rotation to be between 0 and 2π; I will allow any axis, limit the angle to between 0 and π, and invoke crystal symmetry explicitly later. For completeness, we could define cases for which $(\mathbf{u}_1, \theta_1)$ does not yield a CSL,

$$d_{\mathrm{B}}((\mathbf{u}, \theta), (\mathbf{u}_1, \theta_1)) = \infty,$$

except we then need to define the special case $d_{\mathrm{B}}((\mathbf{u}, \theta), (\mathbf{u}_1, \theta_1)) = 0$ if $(\mathbf{u}, \theta)$ is equivalent under symmetry to $(\mathbf{u}_1, \theta_1)$. Making use of the symmetry of the three cubic Bravais lattices (simple, face- or body-centered), we can and should use equivalence classes, and define d_{B} instead to be the Brandon-distance to the nearest CSL: namely, the minimum, over all $(\mathbf{u}^*, \theta^*)$ equivalent to $(\mathbf{u}, \theta)$, of $\Sigma_0^{1/2} \max\{|\theta^* - \theta_1|, \arccos(\mathbf{u}^* \cdot \mathbf{u}_1)\}$.

This Brandon-distance d_{B} is not symmetric: for any two given rotations $d_{\mathrm{B}}((\mathbf{u}_1, \theta_1), (\mathbf{u}_2, \theta_2))$ will usually not be the same as $d_{\mathrm{B}}((\mathbf{u}_2, \theta_2), (\mathbf{u}_1, \theta_1))$, and in fact if one rotation yields a CSL and the other does not, then one d_{B} can be small while the other is infinite. The Brandon -distance d_{B} does not satisfy the triangle inequality (sum of lengths of any two sides of any triangle—including one collapsed to a line segment—is greater than or equal to the length of the third). An example is two rotations that give CSLs, $(\mathbf{u}_1, \theta_1)$ and $(\mathbf{u}_2, \theta_2)$, with $\mathbf{u}_1 = \mathbf{u}_2$ and with both Σ_1 and Σ_2 large, but with there being an angle θ between θ_1 and θ_2 such that the CSL for the rotation about $\mathbf{u}_1$ by θ has a small Σ. The Brandon-distance does satisfy the distance criterion of being non-negative. As for the last criterion, that distance be zero if and only if the two rotations are the same: This criterion holds, because in defining d_{B}, different representations of the same rotation are regarded as the same.

2. Old metallurgist: Brandon used only the first 12 CSLs. If I don't mind going to very large values of Σ, isn't *every* orientation relationship Brandon-close to some CSL?

Young mathematician: That's an interesting question. We can now try to envision as corks on skewers all rotations that are within Brandon-distance $\pi/12$ of some rotation giving a CSL. To do this, instead of thinking of rotations as being given by a pair $(\mathbf{u}, \phi)$, which is in the unit sphere S^2 times the interval $(0, \pi)$, a subset of $\mathbf{R}^3 \times \mathbf{R}^1 = \mathbf{R}^4$, we instead envision rotations as a subset of $\mathbf{R}^3$ by looking at the vectors $\phi\mathbf{u}$ (length ϕ in direction $\mathbf{u}$). The skewer is the ray in direction $\mathbf{u}$. Given a rotation $\phi\mathbf{u}$ yielding a CSL with density Σ, all rotation axes within $\Sigma^{-1/2}\pi/12$ of $\mathbf{u}$ form a cone. The additional requirement that the angle be within $\Sigma^{-1/2}\pi/12$ of ϕ cuts off this cone by caps at angles above and below ϕ by $\Sigma^{-1/2}\pi/12$.

If we represent the rotations in $\mathbf{R}^3$, the Brandon-close rotations to a given rotation look like a tapered cork on a skewer, but one still obtains the Brandon-distance by multiplying the maximum of the angle difference and the axis difference by $\Sigma^{1/2}$—the Brandon-distance isn't ''tapered,'' only the way we represent the rotations. One can handle the equivalent rotations by taking the union over all elements of the cubic symmetry group of each such cork-on-a-skewer. Thus a $\Sigma 5$ cork centered at $\theta = \arctan(1/2)$ on (0,0,1) produces another three corks on that skewer, centered at $\theta + \pi/2$, $\pi/2 - \theta$, and $\pi - \theta$, plus copies of these four on each of the other five equivalent skewers, for a total of 24 equivalent corks. If the axis of rotation is (0,0,1), then there are coincidence site lattices for every pair (h, k) of mutually prime integers. Therefore there is a cork around each point $(0, 0, \arctan(h/k))$ on that skewer. All points on this skewer are inside some cork (in fact, by direct computation, if one includes small angle GBs with angles within $\pi/12$ of zero, each angle between 0 and $\pi/4$ is Brandon-close to one of the following:

$$0, \pi/4, \arctan(1/2), \arctan(1/3), \arctan(2/3), \arctan(3/4);$$

and larger angles of rotation are equivalent to one of these). Your question is whether the union of all the corks, over all rotation axes, completely fills in the solid ball of radius π. Using Brandon's method of measuring the volume of these corks, namely as the area of the spherical cap of axis directions times the range of the rotation angle, the sum of volumes of the corks is infinite, so we know there is lots of overlap. The question (to which I don't know the answer) is whether every point in the ball is in some cork.

3. Old metallurgist: You mention a rotation angle being close to zero degrees. How about such small angle GBs? Brandon's definition requires rotation about any axis be less than 15°. The direction of the rotation axes can be anything and the GB would still be small angle. For any other Σ all three angles matter. How do you resolve this?

Young mathematician: We can just add the Identity, *Id*, to misorientation space, and define $d_{\mathrm{B}}((\mathbf{u}, \theta), Id) = |\theta|$;

once again, we might want to use the minimum of $|\theta^*|$ over all equivalent rotations θ^* $\mathbf{u}^*$ in place of $|\theta|$. (For completion we could also define $d_B(Id, (\mathbf{u}, \theta)) = |\theta|\Sigma^{1/2}$ if $(\mathbf{u}, \theta)$ yields a CSL, and $d_B(Id, (\mathbf{u}, \theta)) = \infty$ if $(\mathbf{u}, \theta)$ doesn't.) In other words, we handle the case of no misorientation (which by extension of the previous parametrization might have been thought of as zero rotation angle about any axis) by just adding a point to misorientation space and defining Brandon-distances to and from it. Note that if we parameterize rotations by the solid ball, then the point added can be taken to be the center of the ball. For a true distance, we would have to make sure the triangle inequality is satisfied, but we already know it is not for the Brandon-distance and so don't worry about it here. In the solid ball representation, now in addition to the corks on skewers we have a ball of radius $\pi/12$ at the center-with the skewers, it is rather like a party presentation of fruit, if we limit to only a few CSLs at least.

4. Old metallurgist: You speak of corks in $\mathbf{R}^3$. Figure 5 in Brandon's paper shows circles on a sphere. How did he manage to lose a dimension?

Young mathematician: For his Fig. 5, Brandon plots ''twinning directions,'' considering rotations that come from picking a normal direction to a plane and obtaining interpenetrating lattices by reflecting the lattice across that plane. Since the space of normal directions is 2-dimensional and the space of all rotations is 3-dimensional, he is only looking at a subset of all possible rotations (using a reflection symmetry of the lattice to convert a reflection into a rotation). Similarly, the notion of distance for that subset, namely the arc length on the sphere from one normal direction to another, is quite different from d_B. You can go from twinning direction to axis–angle by forming the matrix whose first column is the image of the vector (1,0,0) under the reflection, the second is the image of (0, – 1,0), and the third the image of (0,0,1). This is the matrix for the rotation; from it, you can extract axis and angle. For example, his circles for $\Sigma 5$, $\Sigma 13a$, and $\Sigma 17a$ each wind up as four corks on (0,0,1) (and its equivalent axes), while $\Sigma 3$ and $\Sigma 7$ yield corks on (1,0,1).

5. Old metallurgist: I have another question: should the three angles in an orientation relation be given equal weight? There is evidence for a $\Sigma 17$ in tetragonal tin that there are differences when small tilt, twist, or misorientation components are added [2]. Surely there will be similar differences for cubic crystals? For a $\Sigma 3$ twin in fcc, I would expect a big difference between a 5° greater rotation about exact $< 111 >$, and an exact 60° rotation about an axis that is 5° off $< 111 >$.

Young mathematician: Now you are asking about why should one use

$$\Sigma_0^{1/2}\max\{|\theta - \theta_1|, \arccos(\mathbf{u} \cdot \mathbf{u}_1)\}$$

rather than, say, counting closeness of θ more, or misorientation angles differently, or whatever. When you are giving just one number to measure a distance between two things that are inherently 3-dimensional, there will always be such questions. It is a bit like trying to find a metric for how mismatched your clothing is if you wear different color socks and/or different style shoes. The distance you choose to use will depend on the concept you are trying to express.

6. Old metallurgist: Can you give some other examples of parametrizations and metrics used on the space of all rotations?

Young mathematician: As for *Parametrizations*, I've already discussed using axis–angle ($(\mathbf{u}, \theta)$) and the solid ball ($\theta\mathbf{u}$). We've seen some of the advantages and disadvantages of each for visualization. In general, both have multiple representations of the same rotation when the angle is π, as well as multiple rotations equivalent by symmetry, which are rather difficult to compute in these parametrizations.

I also mentioned the common parametrization as a 3×3 matrix A with $AA^T = Id$, $\det(A) = +1$. There are many advantages to such a representation: there is a one-to-one correspondence between such matrices and rotations (thus $SO(3)$ may be used as the notation both for such matrices and for all rotations), they can be determined by finding the images of the coordinate vectors, and composition of rotations is multiplication of matrices. In addition, the set of all matrices which are equivalent to a given matrix can be found by multiplying that matrix by the elements of the symmetry subgroup. A disadvantage is that matrices in $SO(3)$ form a three-dimensional subset of a nine-dimensional space (namely, all 3×3 matrices).

An excellent choice for parametrization is an apparently minor variation in the solid-ball representation $\theta\mathbf{u}$, namely $\sin(\theta/2)\mathbf{u}$. By adding one more number, $\cos(\theta/2)$ to the zeroth position of this triple, one obtains a unit quaternion $\mathbf{e} = \{\cos(\theta/2), \sin(\theta/2)\mathbf{u}\}$ (see, for example, the online encyclopedia wikipedia.org for definitions and usage and [3] for applications in materials science). There are precisely two quaternions, – $\mathbf{e}$ as well as $\mathbf{e}$, to represent each rotation (corresponding to the fact that rotation by θ about $\mathbf{u}$ is

the same as rotation by $2\pi - \theta$ about $-\mathbf{u}$); in defining distances, one always uses the choice giving the smallest result.

Multiplication with quaternions is slightly complicated,[1] but it and other operations with quaternions are part of most mathematical packages for computers. The inverse is simple: replace θ by $-\theta$. The image of a point **p** under the rotation represented by the quaternion **e** is the point **q**, where $\mathbf{e}(0, p_1, p_2, p_3)\,\mathbf{e}^{-1} = (0, q_1, q_2, q_3)$. Composition of rotations parameterized by quaternions **e** and **f** is just quaternion multiplication **ef**. Because quaternions are more efficient for computation, much of the 3D graphics in computer games is done with quaternions.

Finally, one more parametrization sometimes used for rotations is the set of Euler angles: roll, pitch, and yaw. These are more useful for flying airplanes than for materials science.

As for *Metrics* and *Measures*, it is important to realize that the choice of parametrization does not require any particular metric or measure, or vice versa. Any metric can be expressed in any parametrization, although some parametrizations are much easier for describing the physics or for computation using a given metric. For example, if using the θ **u** parametrization, one does NOT want to use the usual metric on $\mathbf{R}^3$; for example, points on opposite sides of the boundary of the ball represent the same rotation! The metric used will determine gradients, and the measure (volume element) will determine densities, proportion of rotations satisfying a given condition, etc. Any time you use or see such quantities, be aware of what metric and measure is being used.

There is a unique (up to scale) measure (volume element) on $SO(3)$ which is invariant under rotations; the same is true for $\mathbf{R}^3$ and the unit sphere S^2 (where the measure is the usual area). To try to estimate what fraction of rotations are close to one of the rotations yielding a CSL with $\Sigma = 19$ or less, Brandon used the measure which is the product of the usual area on the sphere S^2 and the usual length on the circle (quoting from [1] again, ''..the total angular range to be covered, $\pi/6 \times 2\pi$''). This gives a greater amount of weight to angles which are close to zero (small-angle GBs) than if one were to use the invariant measure on $SO(3)$, as Warrington and Boon [4] did. They also count all the rotations equivalent to a given rotation carefully, further explaining the difference between their results and Brandon's. By using an invariant measure in [4], all rotations close to, say, the rotation by angle v about [001] are found by multiplying all rotations appropriately close to the Identity by that rotation. (The set of all rotations near the Identity is a little 3-dimensional chunk of $SO(3)$; multiplying that by the matrix for another rotation gives a little 3-dimensional chunk of $SO(3)$ surrounding that rotation.)

The only rotationally and translationally invariant metric on $\mathbf{R}^3$ is the usual Euclidian distance. There are at least three invariant metrics in common use for the distance between two rotations in $SO(3)$, all based on the angle θ (in $[0, \pi]$) of the rotation Θ resulting from doing one rotation followed by the inverse of the other (the resulting axis doesn't enter into this definition). One is θ itself, another is $2\sin(\theta/2)$, which is the square root of the sum of the squares of the nine entries in the matrix for Θ; it is also given by matrix operations.[2] The third is $2\sin(\theta/4)$, the length of the quaternion which is the difference of the quaternions representing Θ and the identity. The distances are different because the first requires any path between the rotations to stay in $SO(3)$, the second allows the path to go through all matrices, and the third has a naturally different scale parameter, and allows paths to go through all quaternions, not just unit ones. It is perhaps easier to see this for $SO(2)$, where θ is the arc length going around the circle and $2\sin(\theta/2)$ is the length of the chord, which is the distance between the two points as points in $\mathbf{R}^2$. Only the first metric, θ, is what mathematicians call a Riemannian metric on $SO(3)$, as such metrics must use paths which stay in the manifold.

7. Old metallurgist: I now know something about the three angles which characterize an orientation relationship, but five angles are needed to characterize a GB. Don't the other two matter?

Young mathematician: Certainly, and all the issues I've raised concerning parametrizations and metrics on $SO(3)$ apply (even more strongly) to all the angles of grain boundaries. It is easiest to illustrate this with grain boundaries between 2-dimensional grains. Such GBs can be parameterized by the misorientation, which can be given by one angle, and by the normal direction, which can be given by the angle from some specified direction. This space of angles can be parameterized by a rectangle in the plane, with the angle of the normal along the x-axis and the angle of the misorientation along the y-axis. Issues of parametrization versus metric are clear when one makes the analogy to a map of the earth on a rectangle, where longitude is the x-coordinate and latitude the y-coordinate. This is a perfectly good parametrization of the earth

[1] Write $\mathbf{e} = (e_0, \mathbf{v})$ and $\mathbf{f} = (f_0, \mathbf{w})$;
then $\mathbf{ef} = (e_0 f_0 - \mathbf{v}\backslash\mathbf{cdot}\ \mathbf{w}, e_0\mathbf{w} + f_0\mathbf{v} + \mathbf{v}\backslash\mathbf{times}\ \mathbf{w})$.

[2] If A and B are the matrices of the rotations, this is also $\sqrt{3 - \mathrm{trace}(A^{-1}B)} = \sqrt{\tfrac{1}{2}\mathrm{trace}(A-B)(A-B)^T}$.

minus its poles. Longitude is periodic of period 360 degrees, and so one might repeat the map periodically in the x-direction, or might imagine the map being rolled into a tube with the x-axis rolled into the circle representing the equator; similarly for GBs. One would not want to use the usual metric on the plane to determine distances on the earth, except perhaps very locally near the equator. For a metric on grain boundaries, there is absolutely no inherent reason to use the usual invariant distance $\sqrt{(\Delta x)^2 + (\Delta y)^2}$ anywhere in the plane, as misorientation and normal direction are two quite different things, with no symmetry operations mixing them up. A reasonable definition of distance between (θ, θ_n) and (θ^*, θ_n^*) might be the Manhattan metric or its cousins with a relative weight factor w

$$|\theta - \theta^*| + |\theta_n - \theta_n^*| \quad \text{or} \quad \max\{|\theta - \theta^*|, |\theta_n - \theta_n^*|\}$$
$$\text{or} \quad \max\{|\theta - \theta^*|, w|\theta_n - \theta_n^*|\} \quad \text{or} \quad |\theta - \theta^*| + w|\theta_n - \theta_n^*|.$$

Again, one would want to take the minimum over all equivalent (under symmetry operations) GBs. In contrast to the map of the earth, there is periodicity in the misorientation variable as well, so the rectangle should be repeated in the y-direction as well as the x-direction.

8. Old metallurgist: What about low-angle grain boundaries close to the no-boundary limit, as the misorientation approaches zero?

Young mathematician: For interfaces between two difference phases, a boundary between crystals still exists when there is no misorientation; each different normal direction at zero misorientation corresponds to an interface. But for GBs, there is no boundary where there is no misorientation. There are two possible ways to deal with this:

1. Declare it not to be a problem—just as the poles are omitted in the rectangular map of the earth, we can omit the horizontal lines corresponding to the misorientation being 0 (or a multiple of 2π). The fact that quantities such as specific surface free energy γ go to zero as the misorientation approaches zero for any fixed normal direction does not REQUIRE the distances between their angle sets to go to zero. (But such distances will greatly affect gradients!)
2. Compactify the space of grain boundaries by adding a single point called *nil*. Now for any metric, points that are close to *nil* would also have to be close to each other. This is analogous to adding in the poles to the rectangle map of the earth—except that for grain boundaries, one adds only one point *nil* and so the "south pole" would be the same point as the "north pole" and points close to the "south pole" would also be close to the "north pole."

One can try to visualize metrics on the space of 2D grain boundaries in the second way by the shape of the links of an infinitely long linked sausage (though actually each link is the same and all ends of the links are the same point). The sausages could be spherical, similar to copies of the earth placed pole to pole. They could be double-cones, coming to a point at each end. The latter shape would result from using the Manhattan metric, but with the normal angle variable θ_n multiplied by the misorientation angle θ. Or they could be some other shape. Measures can be inferred from these shapes in R^3 (but need not be). The metric and measure could also be more complicated than can be visualized by a surface in $\mathbf{R}^3$.

Symmetries can always be incorporated by replacing actual distances by the minimum among all representatives of the same equivalence class.

There are analogs to all this for grain boundaries in 3D, except the 5-dimensional space is harder to visualize. In particular, one can build a variety of metrics and measures on the space of angles characterizing GB between 3D crystals, including *nil*, based on any metric $d_{SO(3)}$ on $SO(3)$ and any metric $d^3_{\mathbf{R}}$ on $\mathbf{R}^3$. Given GBs $((\mathbf{u}, \theta), \mathbf{n})$ and $((\mathbf{u}', \theta'), \mathbf{n}')$, define $\mathbf{N} = \theta\mathbf{n}$ and $\mathbf{N}' = \theta'\mathbf{n}'$. As examples, one can choose any of

$$d_{SO(3)}((\mathbf{u}, \theta), (\mathbf{u}', \theta')) + d_{\mathbf{R}^3}(\mathbf{N}, \mathbf{N}'),$$
$$\max\{d_{SO(3)}((\mathbf{u}, \theta), (\mathbf{u}', \theta')) + d_{\mathbf{R}^3}(\mathbf{N}, \mathbf{N}')\},$$
$$(d_{SO(3)}((\mathbf{u}, \theta), (\mathbf{u}', \theta'))^2 + d_{\mathbf{R}^3}(\mathbf{N}, \mathbf{N}')^2)^{1/2}.$$

There are also many other possibilities, including different weights. A measure on this space which includes *nil* might be the product of invariant measures on $SO(3)$ and $\mathbf{R}^3$, where one would use $\mathbf{N} = \theta\mathbf{n}$ in place of $\mathbf{n}$ for the $\mathbf{R}^3$ variable. And again, symmetries can incorporated by replacing actual distances by the minimum among all representatives of the same equivalence class.

The ideas I've discussed can be used to analyze a metric proposed by A. Morawiec [5] and used by Saylor et al. [6–8]. Here the misorientation is parametrized by special orthogonal matrices m, and the normal direction by unit vectors $\mathbf{n}$ in $\mathbf{R}^3$. Grain boundaries are then specified by by a 4×4 matrix b, with the upper left 3×3 corner being m, the lower right corner 0, the remainder of the right-most column being $\mathbf{n}$, and the remainder of the bottom row being $\mathbf{n}^T$

m. Define $\chi(b, b')$, the distance from $b := (m, \mathbf{n})$ to $b' := (m', \mathbf{n}')$ by

$$\chi^2(b,b') = ||b-b'||^2/2 = \mathrm{trace}((b-b')^T(b-b'))/2$$
$$= 5 - \mathrm{trace}(m^T m') - \mathbf{n}\cdot\mathbf{n}' - (m^T\mathbf{n})\cdot(m'^T\mathbf{n}')$$
$$= 3 - \mathrm{trace}(m^T m') + 1 - (\mathbf{n}\cdot\mathbf{n}') + 1 - (m^T\mathbf{n})\cdot(m'^T\mathbf{n}').$$

One can observe several properties of this metric. One is that it is straightforward to compute by matrix operations. Another is that the distance does not approach 0 as m approaches m'; rather, $\chi^2\,(m = m') = 2\,(1 - (\mathbf{n}\cdot\mathbf{n}'))$. Therefore, in using this metric to define bins, densities of grain boundaries will appear to be lower for misorientations near the identity as compared to metrics which go to zero as the GBs approach *nil*. Finally, one sees that this metric intertwines **n** and m.

9. Old metallurgist: Let me see if I have your main message straight. There are many possible parameterizations and metrics for hetero-phase interfaces and for grain boundaries in 2D and 3D (2 or 5 angle dimensions). Symmetries can be incorporated into a definition by using a minimization over all grain boundaries equivalent by symmetry to a given boundary. And the ''no boundary'' singularity in GBs might be a clue to appropriate metrics.

Young mathematician: Yes. The rest is up to you, in your choice of metrics and parametrizations.

Old metallurgist: Thank you.

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