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Invited Reply to the Comment
by A Morawiec

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The points raised in Morawiec’s Comment are considered carefully. The question of the shortest distance between two grain boundaries remains unresolved and requires further research.

1. Our criticism of Morawiec's metric

In our paper we sought to separate changes in the boundary parameters associated with the inclination from those associated with misorientation. The impossibility of changing the inclination through changes in the misorientation and vice versa may be seen by considering a spherical grain embedded inside another grain, where the two grains are misoriented. Assign a north pole on the sphere with respect to a fixed laboratory frame; the position of the north pole does not change no matter how the sphere and the surrounding grain are rotated. To change *only* the inclination of the boundary at the north pole we have to *rotate both crystals together*; this operation does not change the misorientation between the crystals. To change *only* the misorientation of the boundary at the north pole we have to *introduce a relative rotation between the sphere and the surrounding grain*. These are distinct operations, and boundaries generated by the first operation cannot be generated by the second and vice versa.

In ref [2] changes in the inclination are effected through changes in the mean boundary plane $\mathbf{N}$. Changes in the misorientation (both axis and angle) are effected through changes in the Rodrigues vector ρ . All possible boundaries with a given misorientation ρ are generated by allowing $\mathbf{N}$ to range over the radius vectors of a sphere¹. This describes the possible boundaries that may surround a grain embedded within another where the misorientation is fixed and the inclination varies. On the other hand by selecting a plane with normal $\mathbf{N}$ inside the perfect crystal and applying equal and opposite rotations of $\theta/2$ to the crystals on either side of the plane about an axis $\hat{\rho}$ we obtain boundaries sharing the same inclination but different misorientations.

In section 5(a) of [2] we noted that Morawiec's metric does not separate these two operations. To achieve this separation we have to replace $(1 - \hat{\mathbf{n}}_1 \cdot \hat{\mathbf{n}}_2) + (1 - \hat{\mathbf{n}}'_1 \cdot \hat{\mathbf{n}}'_2)$ in eqn.(5.1) with $1 - \hat{\mathbf{N}}_1 \cdot \hat{\mathbf{N}}_2$.

Morawiec comments that the separation between contributions from changes in the inclination and misorientation is not a necessary *mathematical* requirement for a function to qualify as a metric. But this misses the point. The point is that the separation is a *physical* requirement because changes in the boundary inclination and misorientation are *independent* since they correspond to distinct operations on the bicrystal.

2. Morawiec's criticism of our metric

Morawiec states that our metric "has the disadvantage that if both the misorientation and the boundary planes are changed in such a way that $\hat{\mathbf{N}}$ is kept constant, only the misorientation change contributes to the growing distance". In eqns (2.1) and (2.2) of ref [2] the boundary normals $\mathbf{n}$ and $\mathbf{n}'$ are *parametrically related* to an arbitrary mean boundary plane normal $\mathbf{N}$ and the Rodrigues vector ρ describing the rotation axis and angle. As we vary the two degrees of freedom associated with the direction of $\mathbf{N}$ and/or the three degrees of freedom associated with ρ the changes in the boundary normals are prescribed by eqns (2.1) and (2.2) of ref [2]. In this way eqns (2.1) and (2.2) define paths through the 5D space. Consequently, it is correct that if $\hat{\mathbf{N}}$ is kept constant while ρ changes then only the change in ρ contributes to our metric. There is no need, and it would be quite wrong, to consider a further contribution to the metric from changes in the boundary normals in this case because those changes have been accounted for already in eqns (2.1) and (2.2).

It should be noted that the information content of eqns (2.1) and (2.2) of ref [2] is exactly the same as that embodied in $\mathbf{n} = \rho \star \mathbf{n}' \star (-\rho) = \mathbf{R}\mathbf{n}'$, where $\mathbf{R}$ is the rotation matrix corresponding to ρ . But the advantage of eqns (2.1) and (2.2) is the explicit vector relationships they provide between the boundary normals and the five degrees of freedom associated with the normal to the mean boundary plane and the misorientation between the adjoining crystals.

¹except at $\theta = \pi$, as discussed here in section 3

3. The limit $\theta \rightarrow \pi$

Morawiec has pointed out limitations in our parameterisation of boundaries in terms of $\mathbf{N}$ and ρ as the misorientation angle $\theta \rightarrow \pi$. In that limit, unless appropriate care is taken, all boundaries described by these equations *appear* to become either pure twist boundaries, with $\mathbf{n}, \mathbf{n}'$ parallel to ρ , or pure tilt boundaries with $\mathbf{n}, \mathbf{n}'$ perpendicular to ρ . In reality there are boundaries at $\theta = \pi$ with their normals at any angle to the rotation axis. They do not appear to be described by eqns (2.1) and (2.2) of ref [2] because as $|\rho| \rightarrow \infty$ either the boundary normals become parallel and anti-parallel to $\mathbf{N} \times \rho$, or they are parallel to ρ if $\mathbf{N}$ is parallel to ρ . This apparent behaviour is illustrated by the example of Morawiec's Appendix A in ref [1].

However, by taking the limit $\theta \rightarrow \pi$ more carefully it is found that eqns (2.1) and (2.2) can describe *all* boundaries in this limit, not only pure twist and pure tilt boundaries. As we stated² between eqns (6.3) and (6.4) of ref [2], at $\theta = \pi$ the boundary normals are related by $\mathbf{n} = 2(\hat{\rho} \cdot \mathbf{n}')\hat{\rho} - \mathbf{n}'$, which indicates that $\mathbf{N}$ is always *parallel* to ρ . It follows that $|\mathbf{N} \times \rho| \rightarrow 0$ as $\theta \rightarrow \pi$, in contrast to the previous paragraph where it appeared that $|\mathbf{N} \times \rho| \rightarrow \infty$ as $\theta \rightarrow \pi$.

As θ approaches π the boundary normals are related by $\mathbf{n} = 2(\hat{\rho} \cdot \mathbf{n}')\hat{\rho} - \mathbf{n}' - 2\mathbf{n}' \times \hat{\rho}/|\rho|$. Then we have:

$$\mathbf{N} = (\hat{\rho} \cdot \mathbf{n}')\hat{\rho} - \frac{\mathbf{n}' \times \hat{\rho}}{|\rho|} = (\hat{\rho} \cdot \mathbf{n})\hat{\rho} + \frac{\mathbf{n} \times \hat{\rho}}{|\rho|} \tag{3.1}$$

If these expressions for the mean boundary plane $\mathbf{N}$ are substituted into eqns (2.1) and (2.2) of ref [2] we find they are satisfied identically for *any* orientation between $\mathbf{n}$ and $\hat{\rho}$ as $\theta \rightarrow \pi$. But since the mean boundary plane converges to the rotation axis for all boundaries the mean boundary plane no longer distinguishes between boundary planes sharing the same rotation axis in the limit $\theta \rightarrow \pi$. Instead the distance between two boundaries sharing the same $\hat{\rho}$ at $\theta = \pi$ is the angle $\cos^{-1}(\hat{\mathbf{n}}_1 \cdot \hat{\mathbf{n}}_2) = \cos^{-1}(\hat{\mathbf{n}}'_1 \cdot \hat{\mathbf{n}}'_2)$.

The central issue here is that at $\theta = \pi$ the mean boundary plane normal and the rotation axis are parallel. Eqns (2.1) and (2.2) of ref [2] still apply in this limit if the correct limiting behaviour of the mean boundary plane in eqn 3.1 is observed, as indeed they must. But at $\theta = \pi$ one has to use either $\hat{\mathbf{n}}$ or $\hat{\mathbf{n}}'$ instead of the mean boundary plane normal as the two degrees of freedom associated with the boundary plane. It is a weakness of our approach that the mean boundary plane ceases to distinguish between boundaries sharing the same rotation axis at $\theta = \pi$.

4. Symmetry

Symmetry-related descriptions of a boundary are descriptions of the same physical reality. This leads Morawiec in eqn (1) of ref [1] to require that the distances between equivalent descriptions of two boundaries are the same. He has met this requirement in ref [3] by *defining* the Hausdorff distance between the two sets of points representing equivalent descriptions of two boundaries. The Hausdorff distance is the maximum distance of a point in either set to the nearest point in the other set. In this way Morawiec satisfies the 4 requirements of a metric listed in section 4 of ref [2] and eqn (1) of ref [1] - a unique achievement as far as I know.

In ref [2] we asked a different question, one that has been implicit throughout the history of research on grain boundaries. It concerns the *shortest path* in the 5D parameter space between two grain boundaries, as defined by the smallest sum of rotation angles required to map one boundary onto another, involving changes in both inclination and misorientation in general. The shortest path is needed to interpolate a physical property of the boundary core between two boundaries where the property has been determined, such as diffusivity or tendency for equilibrium segregation of some impurity. The shortest path is not the Hausdorff distance.

Our approach to answering this question is to examine the distance between every pair of points in the two sets of equivalent representations, regarding them as distinct even though

²There is a typographical error in this section: $2(\hat{\rho}_2 \cdot \mathbf{n})\hat{\rho}_2 - \mathbf{v}$ should be $2(\hat{\rho}_2 \cdot \mathbf{v})\hat{\rho}_2 - \mathbf{v}$.

the points in each set are equivalent representations. The justification for this approach is that it should enable us to identify the shortest path between the two sets of points.

Morawiec points out that in general our approach violates the triangle inequality: once the shortest path $\mathcal{P}$ has been identified between the sets of points in the 5D space representing two boundaries there may be an even shorter path that involves passing through some representation(s) of a third boundary not on $\mathcal{P}$. This is a fascinating observation and it raises a number of questions for further research. For example, how does one find the shortest distance between two boundaries allowing for the possibility of violations of the triangle inequality involving a third boundary, and is there an upper bound on the shortest direct path between points representing two boundaries before the triangle inequality is violated by involving a third boundary?

5. Conclusions

- (i) A metric for grain boundaries must distinguish between (a) changes in the boundary inclination and (b) changes in the boundary misorientation. This is a *physical* requirement because changes in one cannot be effected by changes in the other. Morawiec's metric does not appear to satisfy this requirement.
- (ii) In the limit that the boundary misorientation angle $\theta \rightarrow \pi$ the limiting behaviour of the mean boundary plane has to be treated with care to avoid the erroneous conclusion that all boundaries are either pure tilt or pure boundaries at $\theta = \pi$.
- (iii) When $\theta = \pi$ the mean boundary plane does not distinguish between different inclinations. In that case either boundary normal may be used instead of the mean boundary plane.
- (iv) By using the Hausdorff distance Morawiec's metric satisfies all the requirements of a metric as well as the very reasonable requirement that the distances between symmetry-related representations of two boundaries are the same. However, the Hausdorff distance is not the smallest distance between two boundaries. It is therefore inappropriate to use this metric for interpolation of a property of the cores of boundaries between two boundaries where the property is known.
- (v) In general the metric proposed in ref [2] violates the triangle inequality, which invalidates it as a metric. It is not clear whether the shortest distance between two boundaries can ever satisfy the requirements of a metric.
- (vi) The question of the shortest distance between two boundaries, by which we mean the smallest sum of rotation angles required to map one boundary onto another, remains unresolved and requires further research.

Ethics statement. I regret that at the time of writing ref [2] we were unaware of [3], which is a key paper in the field.

Data accessibility. There are no data in this paper.

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Conflict of interests. I declare that I have no conflicts of interest.

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