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# Representation of single-axis grain boundary functions

Srikanth Patala [a,b,*], Christopher A. Schuh [a]

[a] Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
[b] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

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**Abstract**

The ability to describe continuous functions on the space of grain boundary parameters is crucial for investigating the functional relations between the structure and the properties of interfaces, in analogy to the way that continuous distribution functions for orientations (i.e. texture information) have been used extensively in the optimization of polycrystalline microstructures. Here we develop a rigorous framework for the description of continuous functions for a subset of the five-parameter grain boundary space, called the "single-axis grain boundary" space. This space consists of all the boundary plane orientations for misorientations confined to a single axis, and is relevant to the method of presenting boundary plane statistics in widespread current use. We establish the topological equivalence between the single-axis grain boundary space and the 3-sphere, which in turn enables the use of hyperspherical harmonics as basis functions to construct continuous functions. These functions enable the representation of statistical distributions and the construction of functional forms for the structure–property relationships of grain boundaries.


*Keywords:* Grain boundaries; Crystal symmetry; Grain boundary planes; Distribution functions

## 1. Introduction

The importance of grain boundaries to the properties of polycrystalline materials is widely appreciated and is quickly becoming a cornerstone of the modern materials design paradigm. There are numerous instances where grain boundary distributions have been manipulated to improve the functional and mechanical properties of polycrystalline materials [1–8]. While the primary focus of many of these studies has been to tailor the grain boundary misorientations, there has been a recent emphasis on manipulating the grain boundary plane distributions to obtain better properties [9–13]. These investigations have benefited greatly from experimental advances in the characterization of grain boundaries in full crystallographic detail, inclusive of all five macroscopic parameters defining their geometry [14–19]. The focus for the future of grain boundary engineering is shifting towards simultaneously tailoring the five parameters.

One significant obstacle to the investigation of the distributions of the five grain boundary parameters is a lack of analytical tools to describe the distributions of quantities involving both the misorientation and the boundary-inclination aspects of grain boundaries. This is because the five-parameter space is vast and has a complicated topology due to various constraints. Owing to symmetries of the boundary and the crystals abutting it, there are some duplicate sets of distinct parameters that describe the same physical boundary, and hence are symmetrically equivalent. Such symmetry constraints can be expressed as equivalence relations, and have been developed in detail elsewhere [20–22]. It is useful to reiterate these here:

$$(M;\vec{n}) \sim \left((S^i)^{-1} M (S^j); \mathbf{g}\left[(S^i)^{-1}\right] * \vec{n}\right) \quad \text{where } i, j \in \{1,\ldots,n\} \tag{1a}$$

$$(M;\vec{n}) \sim (M^{-1}; \mathbf{g}[M^{-1}] * (-\vec{n})) \tag{1b}$$

$$(I;\vec{n}) \sim (I;\vec{n'}) \quad \forall \vec{n}, \vec{n'} \in S^2 \tag{1c}$$

* Corresponding author at: Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA.
*E-mail address:* srikanth.patala@gmail.com (S. Patala).

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In these expressions, $M$ denotes the misorientation, $\vec{n}$ represents the boundary-plane normal vector, and $S$ represents a point symmetry operation of the crystallographic point group of order $n$. The operation $\mathbf{g}$ simply outputs the $3 \times 3$ matrix equivalent to the rotation operation in its argument, regardless of the parameterization used. $I$ represents the identity matrix corresponding to the zero-misorientation angle. These three equivalence relations capture some important physical concepts about grain boundary crystallography: (i) rotating one or both of the crystals through one of their symmetry operations does not change the boundary; (ii) the boundary is physically the same when viewed from either of the two grains at the boundary (the "grain exchange symmetry"); and (iii) if there is no misorientation, then there is no unique boundary plane either (the "no-boundary singularity").

To be able to analyze and exploit the full potential of the vast amounts of grain boundary data that can now be obtained from microstructural analysis, it is crucial to develop tools that help resolve or remove some of the complexities of the grain boundary space. This is largely an open problem at present [23]. In Ref. [24], we addressed a simple version of the problem, for one-dimensional boundaries between two-dimensional (2-D) crystals. By appropriately transforming the 2-D grain boundary parameters, the no-boundary singularity was resolved, and by including the grain exchange symmetry, the space of grain boundary parameters was shown to be equivalent to the 2-sphere with appropriate equivalence relations ($S^2/E$). The analysis of the 2-D grain boundary space emphasized the necessity of a new parameterization that naturally accounts for the no-boundary singularity and simplifies the equivalence relation associated with the grain exchange symmetry.

In this paper, we present developments that resolve a subset of the five-parameter grain boundary space, the single-axis grain boundary (SAGB) space. The SAGB space is the collection of grain boundary parameters with the misorientation axis confined to lie along any specific crystal direction $\vec{b}$ (with certain exceptions discussed in Section. 2). This subset of the complete grain boundary space is particularly relevant because, in the experimental literature, grain boundary planes are often analyzed for misorientations along a specific symmetry axis of the crystal [25–31]. This space also describes the collection of grain boundaries of perfect fiber-textured materials, and has direct relevance to, for example, thin films and severely extruded metals.

## 2. Mapping the single-axis grain boundary space onto the hypersphere ($S^3$)

As mentioned previously, the SAGB space is the collection of all boundary-plane orientations corresponding to disorientations (i.e. the misorientations lying in the fundamental zone of interest) along a fixed crystal direction $\vec{b}$. The boundary inclination space is the unit-sphere in three dimensions (2-sphere, $S^2$) since any normal vector can be represented as a point on the unit-sphere. Therefore, from a topological perspective the SAGB space is the product space $[0, \omega_{\max}] \times S^2$, where $\omega_{\max}$ is the maximum disorientation angle along the axis $\vec{b}$ in the fundamental zone. More precisely, the SAGB space is equivalent to $[[0, \omega_{\max}] \times S^2]/E$, where $E$ is the equivalence class representing all possible symmetries of the boundary-plane spaces (i.e. Eq. (1)). In Ref. [22], we have enumerated these symmetries for disorientations belonging to all the crystallographic point groups.

The first objective of this article is to find a suitable transformation of the boundary parameters that maps the SAGB space ($[[0, \omega_{\max}] \times S^2]/E$) to the 3-sphere $S^3$ (with coordinates $(x_1, x_2, x_3, x_4)$ in $\mathbb{R}^4$ such that $\sum_{i=1}^{4} x_i^2 = 1$) with a convenient set of equivalence relations. Before considering these mappings and symmetries in detail, certain conventions are introduced. The symmetries of the boundary-plane spaces are denoted by $G$. As observed in Ref. [22], when $\omega$ belongs to the interval $(0,\omega_{\max})$, all the boundary-plane spaces $S^2$ exhibit symmetries of a single point group (denoted as $G_1$) and we denote the symmetries of the boundary-plane space when $\omega = \omega_{\max}$ as $G_2$ (where $G_1 \subseteq G_2$). In this paper, the quaternion ($\mathbf{q}$) parameterization is used to represent misorientations ($M$) and the grain boundary parameters are hence denoted as $(\mathbf{q};\vec{n})$. The mapping of the $(\mathbf{q},\vec{n})$ parameters to the 3-sphere is obtained through the following steps:

(a) The first equivalence relation that needs to be addressed is that of the no-boundary singularity Eq. (1c), which is crucial to the mapping between the product space $[0, \omega_{\max}] \times S^2$ and $S^3$. According to this singularity, the space $S^2$ corresponding to the zero misorientation angle needs to be collapsed to a single point. This is achieved by the following mapping from the $(\mathbf{q};\vec{n})$ to the $(\mathbf{q};\vec{r})$ parameterization:

$$(\mathbf{q};\vec{r}) = C(\mathbf{q};\vec{n}) = (\mathbf{q};[C(\mathbf{q}) * \vec{n}]) \tag{2}$$

where $C(\mathbf{q})$ is a scalar function defined as:

$$C(\mathbf{q}) = \sqrt{1 - \max\{((\mathbf{q} * \mathbf{G})_0)^2\}} \tag{3}$$

$\mathbf{G}$ is the point group symmetry of the crystal. $\mathbf{q} * \mathbf{G}$ is the left co-set of $\mathbf{G}$ in $SO(3)$ and $(\mathbf{q} * \mathbf{G})0$ is the set of the first quaternion components of the left co-set $\mathbf{q} * \mathbf{G}$. To state it simply, $C(\mathbf{q})$ is a continuous function on the quaternion space and takes the value zero when the boundary misorientation is either the identity or symmetrically equivalent to the identity. In the case of the grain boundary space of a crystal with rotational point group symmetry $C_1$, $\mathbf{G} = C_1 = \{I\}$, $(\mathbf{q} * \mathbf{G})_0 = q_0$ and thus $C(\mathbf{q}) = \sqrt{1 - q_0^2}$. In general, for all crystallographic point groups, $C(\mathbf{q}) = \sqrt{1 - q_0^2} = \sin\left(\frac{\omega}{2}\right)$ if $\mathbf{q}$ belongs to the fundamental zone.This mapping results in a parameterization $(\mathbf{q};\vec{r})$ that is compatible with the no-boundary singularity by collapsing all the boundary normal vectors corresponding to the zero misorientation angle to