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The uncorrelated triple junction distribution function: Towards grain boundary network design

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Abstract

Triple junctions are recognized as important microstructural features in the context of grain boundary network topology and grain boundary sensitive materials properties. In spite of this prominence, mathematical tools for quantifying distributions of misorientations around triple junctions have been limited to special cases. Here we derive a general formula for the uncorrelated triple junction distribution function (TJDF) for materials of arbitrary texture. Additionally, we provide the mathematical link between TJDF and the orientation distribution function, which should facilitate the use of materials design paradigms on the grain boundary network.

Keywords: Triple junction; Triple junction distribution function; Microstructure design; Grain boundary engineering

1. Introduction

Grain boundary engineering (GBE) techniques have demonstrated the potential for dramatic materials properties enhancement; in some cases, improvements of more than an order of magnitude have been observed [1–4]. While such studies have empirically demonstrated the enhancement of materials properties through manipulation of the grain boundary network, a theory for the design of microstructures with optimized grain boundary networks is still lacking. Fig. 1 schematically illustrates the current state of the art in microstructure characterization, materials properties prediction and materials design. For materials properties that are sensitive to crystallographic orientation, the rigorous mathematical tools of texture analysis and homogenization theory provide the underpinning methodology to address the forward problem of predicting effective macroscopic properties. These techniques are detailed in the seminal work by Bunge [5]. The inverse problem of designing a microstructure with a specified effective macroscopic materials property has also been treated for orientation dependent properties thanks to the Microstructure Sensitive Design for Performance Optimization formalism developed by Adams et al. [6].

However, the materials properties that are most likely to be enhanced by GBE are dominated, not by the orientation of grains, but rather by the misorientation of grain boundaries and their spatial arrangement within the grain boundary network. Examples include intergranular fracture [7], intergranular corrosion [8] and liquid metal embrittlement [9,10]. For such network-dominated properties as these, neither the forward problem of properties prediction nor the inverse problem of materials design has been solved, and a fundamental framework on which to approach a solution does not even exist. It is this gap in the literature that the present work attempts to address.

The improvement in properties that has been achieved through GBE has been ostensibly linked to an increase in the population of certain "special" grain boundaries [1,2,4,11–14], e.g. low-angle or coincidence site lattice (CSL) boundaries. However, it is known that grain boundary networks in real materials are not, and in fact never can be, randomly assembled, due to the existence of certain

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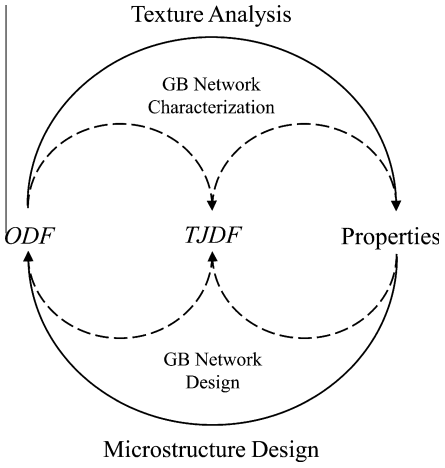

Fig. 1. Schematic illustration showing the gaps in the microstructure design literature (dotted lines). Much work has focused on prediction of properties that depend on texture (solid lines). This is typically done by using the ODF in homogenization relations. However, much less has been done in the realm of property prediction or materials design when the properties of interest are dependent on the misorientations of grain boundaries and their spatial distribution in the grain boundary network. This work attempts to fill this gap by making an explicit connection between the ODF and the TJDF.

crystallographic constraints [15–35]. Such spatial arrangement issues have been studied heavily [7,19,21,26,32,36–40], and are strongly linked to, e.g., triple junction types [26,32]. It has also been noted that the constraints imposed by higher order topological features of the microstructure play a decreasingly significant role [41]. Thus, it would appear that triple junctions occupy a unique position in the hierarchy of topological descriptors: they are the simplest microstructural component that encodes sufficient topological information to characterize the major features of real grain boundary networks. Additionally, triple junctions play the unique role of decision points or hubs for the transmission of various forms of intergranular damage. Depending upon the specific crystallography of a triple junction, it may either impede or permit the propagation of an incident crack (for example). The triple junction thus emerges as a key feature of the grain boundary network, constraining the assembly of grain boundaries, controlling (to a large degree) the long-range connectivity of boundaries of specific types and regulating the flow of various damage processes.

Accordingly, we envision a materials design paradigm for GBE materials as comprising tools like those described for texture control, with triple junctions at the center (see Fig. 1). Just as in texture analysis, where the orientation distribution function (ODF) is the weighting function that allows one to compute average or "effective" properties, the triple junction distribution function (TJDF) could serve a similar purpose for homogenization over the grain boundary network. With tools to connect texture to triple junctions, and triple junctions to properties, one can envision an approach to the inverse problem. It is our purpose in this paper to present the TJDF as the central component in this design paradigm, as illustrated in Fig. 1.

While various researchers have studied the theoretical aspects of grain boundary networks (see e.g. [28,31,42–44]), the concept of the TJDF has only been touched upon in a relatively limited way. For example, Mason derived the TJDF for the case of crystallographically consistent grain boundary networks with perfect in-plane textures [28], and both Mason and Frary independently derived the triple junction fractions for the same specific case [18,28]. Hardy and Field considered the TJDF for the special case where triple junctions are composed of at least one coherent twin boundary [45,46].

In the present work, we derive a general formula for the uncorrelated TJDF of materials possessing arbitrary texture. We also provide a mathematical relation that links the TJDF to the ODF. This result connects our work to the existing body of microstructure design literature (e.g. [5,6,47,48]), and should facilitate solution of the inverse problem through a texture-based approach to grain boundary network design. The present work thus lays mathematical groundwork necessary for the design of grain boundary networks.

2. Conventions

In this paper we follow the active rotation convention, as in Ref. [49]. This treatment regards a rotation operation as an active transformation of the points of configuration space, with respect to a right-handed orthonormal set of space-fixed axes. From this point of view a crystal orientation is defined as the rotation which, when applied to the coordinate system of a reference crystal, brings it into coincidence with the coordinate system of the oriented crystal. All such rotations belong to the proper rotation group, $SO(3)$, and can be defined by three independent parameters. In this paper we use the quaternion parameterization of $SO(3)$. Explicitly, the components of a unit quaternion, $q = [a, b, c, d]$, are related to elements of $SO(3)$ by [49]:

$$\begin{aligned} a &= \cos(\omega/2) \\ b &= \sin(\omega/2)\sin\theta\cos\phi \\ c &= \sin(\omega/2)\sin\theta\sin\phi \\ d &= \sin(\omega/2)\cos\theta \end{aligned} \tag{1}$$

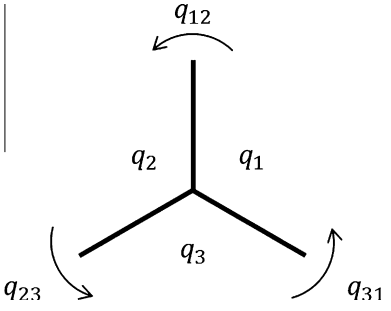

Fig. 2. Schematic triple junction illustrating the nomenclature used in this paper for grain orientations, q_i, and grain boundary misorientations, q_{ij}.