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The triple junction hull: Tools for grain boundary network design

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ABSTRACT

Grain boundary engineering (GBE) studies have demonstrated significant materials properties enhancements by modifying the populations and connectivity of different types of grain boundaries within the grain boundary network. In order to facilitate rigorous design and optimization of grain boundary networks, we develop theoretical tools that are based upon a spectral representation of grain boundary network statistics. We identify the connection between a local length scale, embodied by triple junctions, and a global length scale, associated with the grain boundary network configuration as a whole. We define the local state space for triple junctions, $\mathcal{A}^{(3)}$, and enumerate its symmetries. We further define the design space for grain boundary networks, $\mathcal{M}_H^{(3)}$, characterize its important geometric properties, and discuss how its convexity permits grain boundary network design. We also investigate the extent to which the control of texture alone allows one to probe the full design space.

1. Introduction

In the context of texture and grain structure in polycrystalline materials, microstructure design tools now allow the designer to explore a complete set of physically realizable microstructures and identify those that meet various performance objectives and design constraints (Adams et al., 2001, 2012). These tools have been used to address design problems in which elastic and plastic properties are concerned (Adams et al., 2001; Fast et al., 2008; Houskamp et al., 2007; Kalidindi and Houskamp, 2007; Kalidindi et al., 2004; Lyon and Adams, 2004; Saheli et al., 2005; Sintay and Adams, 2005). However, their application to other properties of scientific and engineering interest, such as fracture and corrosion, which depend upon the structure of the grain boundary network, remains to be addressed. This is an area of great opportunity because grain boundary engineering (GBE) studies have demonstrated significant enhancements of materials properties (Lehockey and Palumbo, 1997; Lehockey et al., 1998a,b, 1999; Norton et al., 1996), but there is currently no "inductive" method (Olson, 1997) by which to design such successes *a priori*. For instance, Lin et al. (1995) observed a two-fold decrease in the intergranular corrosion rate of Alloy 600 after GBE processing (Lin et al., 1995). However, no major change in texture accompanied this enhancement in properties. Characteristic of GBE materials, the resultant texture was nearly random, but contained a high fraction of low-energy grain boundaries (up to 55% of the boundaries were Σ3 type). Contrast this with the fact that for a microstructure with uncorrelated grain orientations and random texture the expected population of such boundaries is extremely small (~1.8%) (Morawiec et al., 1993). It would appear, then, that texture is insufficient to explain or predict such materials properties enhancements and, consequently, design tools that incorporate the character and connectivity of the grain boundary network are needed.

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In previous work, we introduced a general triple junction distribution function (TJDF) as the core of a design strategy for grain boundary networks (Johnson and Schuh, 2013). The TJDF provides a statistical description of grain boundary network connectivity that facilitates adaptation of the existing design framework to grain boundary network design. Expressed in the context of the spectral framework of Johnson and Schuh (2013), the TJDF provides a bridge between crystallographic texture and grain boundary network topology. These tools allow one to rigorously bound the universe of all possible grain boundary network configurations. In this work, we employ our previous results in order to define the triple junction hull, $\mathcal{M}_H^{(3)}$, which constitutes the first order design space for grain boundary networks. $\mathcal{M}_H^{(3)}$ bounds the entire space of physically realizable grain boundary networks, and is pivotal for the adaptation of existing tools to the problem of grain boundary network design. We also investigate the relative size of the subspace of $\mathcal{M}_H^{(3)}$ that is accessible through the control of crystallographic texture alone.

2. Triple junction state space

Grain boundary network design is an intrinsically multi-scale endeavor, requiring the practitioner to specify both (1) the local state and (2) the spatial location of grain boundaries within the network. However, real grain boundary networks

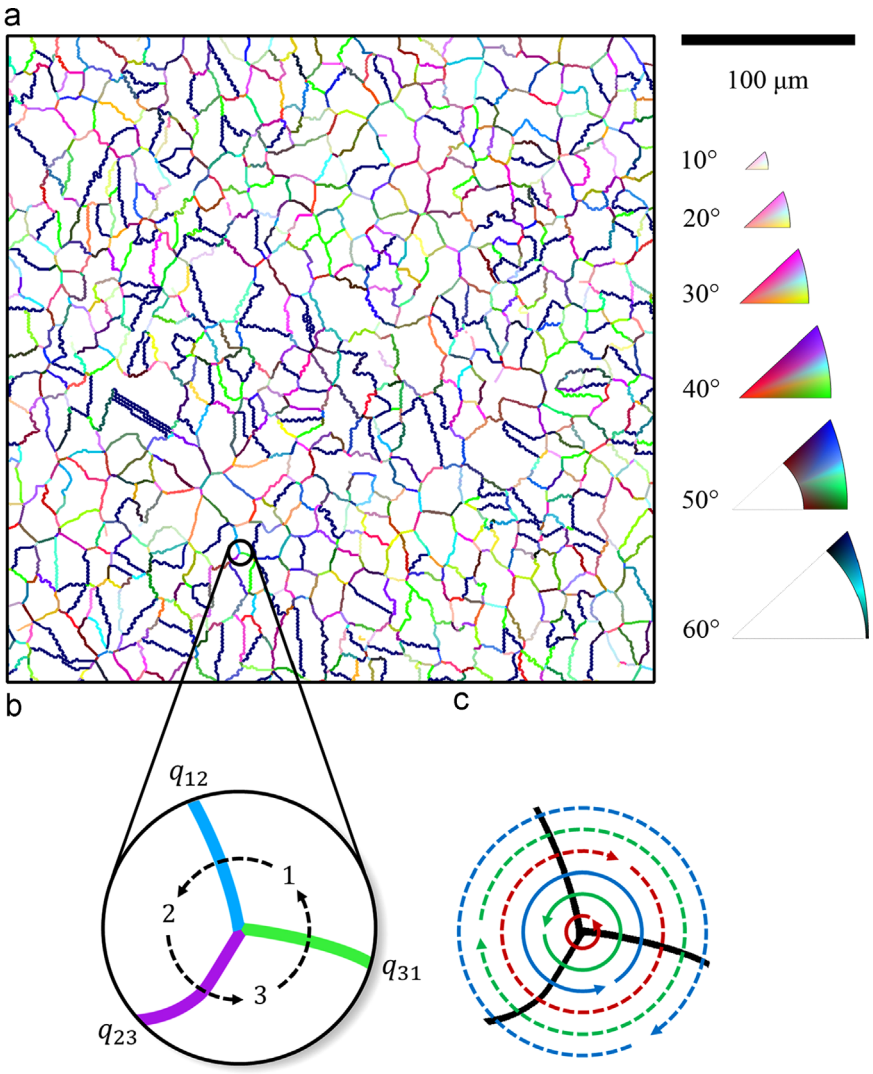

Fig. 1. (a) The grain boundary network of a sample of Inconel 690, representing a global configuration of triple junctions. Grain boundaries in (a) are color coded by their disorientation axis (in the standard stereographic triangle) and angle (see the legend at right) (Patala et al., 2012). (b) The local state of a representative triple junction as indicated by its grain boundary misorientations, q_{AB}. The grains coordinating the triple junction are labeled 1, 2, and 3, with dotted arrows defining a circuit that encloses it. Composition of the grain boundary misorientations around such a circuit must result in the identity operation (Eq. (3)). (c) All six distinct paths surrounding a triple junction. These correspond to all possible ways of choosing the two independent misorientations coordinating a triple junction, and thus, represent physically equivalent descriptions. Colors distinguish circuits starting in different grains, and line type (solid/dashed) distinguish circuits of different sense. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)