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Quadruple nodes and grain boundary connectivity in three dimensions

S.F. Li[a,*], J.K. Mason[a,b], J. Lind[c], M. Kumar[a]

[a] Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
[b] Boğaziçi University, Bebek, Istanbul 34342, Turkey
[c] Carnegie Mellon University, Pittsburgh, PA 15213, USA

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Abstract

Recent high-energy diffraction microscopy experiments allow a microstructure to be reconstructed as a 3-D volume mesh at a resolution significantly smaller than the characteristic grain size. This presents an opportunity to evaluate the performance of the stereological predictors of the distribution of quadruple node types. The reconstructed microstructures of two materials with different processing histories are found to contain different distributions of quadruple node types, and provide reference points for a comparison of the stereological predictors. While none of the predictors considered here is completely satisfactory, one based on the examination of triangular grains on planar sections and one based on the identification of topological transitions in the grain boundary network on adjacent planar sections perform well enough to be of some practical use. Some of the sources of statistical and systematic error that cause the predictors to deviate from the observed distribution of quadruple node types are explored, and the Hellinger distance is proposed as a means to compare distributions of quadruple node types in practice.

Keywords: Stereology; Diffraction; 3D microstructure

1. Introduction

The tetrakaidecahedron shown in Fig. 1a is often considered to be a good representative of the geometry of the grains in a typical material microstructure [1–3]. This polyhedron may be periodically repeated to fill space, with the resulting configuration satisfying the topological requirements that two grains meet on a face, three faces meet on a triple line, and four triple lines meet on a quadruple node. Furthermore, Lord Kelvin's prediction [3] that this is the unique space-filling periodic structure with minimal surface area encourages the use of tetrakaidecahedra for models of physical systems with an interfacial energy per unit area, e.g. for the grain boundary network in a material microstructure. Although Lord Kelvin's conjecture is now known to be false [4], the simplicity and symmetry of the tetrakaidecahedron continue to make this polyhedron appealing as a model for grain geometry.

Particularly with regard to stereology, or the interpretation of a 3-D structure from planar sections, the assumption that a grain is well represented by a convex polyhedron with planar facets may not be suitable for many microstructures. Consider the grain shown in Fig. 1b, reconstructed by high-energy diffraction microscopy (HEDM) experiments on high-purity Cu. The complex morphology of this grain indicates that, for example, identifying the number of distinct grains in a single 2-D planar section of this microstructure, as in Fig. 1c, would require detailed knowledge of the grain connectivity in three dimensions.

For precisely this reason, practical stereology is often restricted to geometric features (e.g. the volume or surface

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* Corresponding author.

E-mail addresses: li31@llnl.gov (S.F. Li), jeremy.mason@boun.edu.tr (J.K. Mason), jlind@andrew.cmu.edu (J. Lind), kumar3@llnl.gov (M. Kumar).

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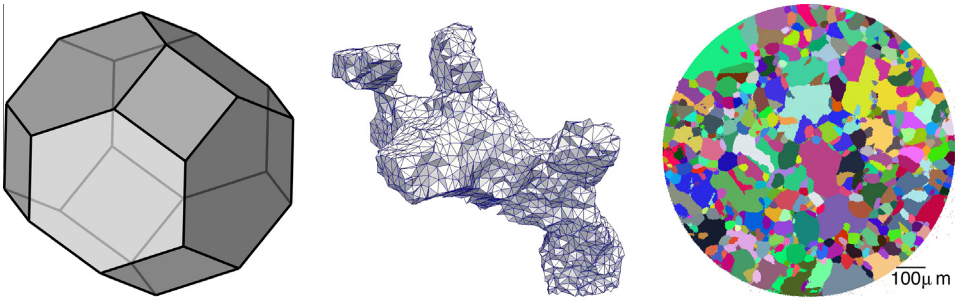


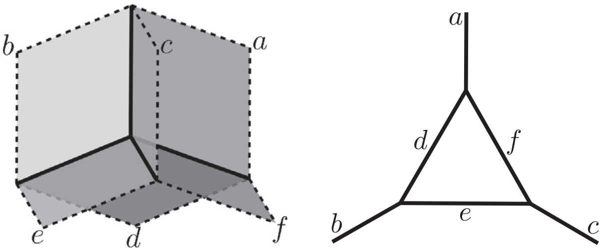
(a) Tetrakaidecahedron (b) Physical grain (c) GBE Microstructure

Fig. 1. (a) The tetrakaidecahedron is often considered to be representative of a typical grain. (b) By comparison, physical grains are often non-convex and do not have planar facets. (c) A typical cross-section of a grain boundary engineered Cu sample.

area of a second phase) rather than topological features (e.g. the number density of particles) of the microstructure [5,6]. Nevertheless, there are indications [7–13] that the topological characteristics of the grain boundary network strongly influence the material response. Consider the failure of a 2-D material by intergranular fracture. Whenever the crack front propagates across a grain boundary and arrives at a triple junction, there is the opportunity for the crack to be arrested if the two adjoining boundaries are sufficiently resistant to fracture [14–18,12,19,20]. Hence, the frequencies of triple junction types regulate the connectivity of a 2-D grain boundary network. Since the analogous 3-D topological feature is the quadruple node, the frequencies of quadruple node types presumably regulate the connectivity of the 3-D grain boundary network [21–24] and the resulting material response.

Despite this, quadruple nodes are mentioned relatively infrequently in the literature. One reason may be that quadruple nodes have the dimensionality of a point and do not intersect generic planar sections of the microstructure, making direct observation difficult. This likely motivated the development of a stereological technique to measure the frequencies of quadruple node types by Frary [25], based on the taxonomy given in Frary and Schuh [24]. Specifically, the frequency of a type of quadruple node is indicated by Q_{ij}, where i is the number of incident special boundaries and j is the number of incident triple lines coordinated by at least two special boundaries. Within this study, a special boundary is defined as a coincident-site-lattice (CSL) boundary [26] with $\Sigma \leqslant 29$ [27], to within the tolerance of the Brandon criterion [26]. Frary [25] suggested that the Q_{ij} could be estimated from the arrangement of grain boundaries appearing around triangular grains in a single planar section, roughly identifying the grain boundaries around the triangular grain with those around a quadruple node as indicated in Fig. 2.

As justification for this technique, Frary [25] observed that the crystallographic constraints on the types and arrangement of grain boundaries around a quadruple node are identical to those around a triangular grain in a planar section. While true, this does not account for energetic or kinetic effects that may favor the stability of certain quadruple node configurations over others, meaning that the presence of identical crystallographic constraints is not a sufficient condition for the measured and estimated quadruple node frequencies to be the same. Indeed, the close correspondence of the measured and estimated quadruple node frequencies reported by Frary [25] may be attributed to the use of simulated microstructures that contained exclusively convex grains, with the result that the majority of triangular grains in a planar section actually correspond to quadruple nodes in the 3-D microstructure.



(a) Quadruple node (b) Corresponding triangular grain

Fig. 2. (a) The configuration of four grains, six grain boundaries, and four triple lines around a quadruple node. (b) The corresponding triangular grain in a planar section that intersects the configuration in (a) just below the quadruple node. The grain boundary labels in (a) correspond to those in (b).

The purpose of this paper is to investigate the performance of various stereological predictors of quadruple node frequencies in real microstructures containing grains with arbitrarily complicated morphologies. This is accomplished by using HEDM measurements to make a 3-D reconstruction of the microstructure, and employing the quadruple node frequencies of the reconstructed surface mesh as a reference distribution. We apply the stereological predictors directly to planar sections from the HEDM measurements, and extensively analyze the statistical and systematic errors that make the predictors deviate from the expected distribution. All of the predictors (including the one proposed in Section 3.2) are found to exhibit some form of systematic bias, stressing the difficulty of understanding 3-D microstructural features from observations of 2-D sections.

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