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Comparative grain topology

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Abstract

Space-filling polyhedral networks are commonly studied in biological, physical, and mathematical disciplines. The constraints governing the construction of each network varies considerably under each context, affecting the topological properties of the constituents. A method for mapping the topological symmetry of a space-filling population of polyhedra is presented, relative to all possible polyhedra. This method is applied to the topological comparison of populations generated by seven different processes: (i) natural grain growth in polycrystalline metal, ideal grain growth simulated by (ii) interface-tracking and (iii) phase-field methods, (iv) Poisson–Voronoi and (v) ellipsoid tessellations, and (vi) graph-theoretic and (vii) Monte Carlo enumerations of individual polyhedra. Evidence for topological bias in these populations is discussed.

Keywords: Computer simulation; Grain growth; Microstructure; Topology; Phase-field method

1. Introduction

In polycrystalline metals, physical properties such as tensile strength, ductility and creep resistance depend strongly on microstructure: the nature and proportions of constituent elements or phases on microscopic length scales. Metrical properties, especially grain radii, have long been studied; through stereology, simple measurements are used to accurately estimate physical behavior. Topological properties and their influence on physical properties is less completely understood, although topology features prominently in the kinetics of grain boundary motion in two and three dimensions [1–3].

In 1887, Lord Kelvin conjectured that, to fill 3-D space with identical cells, the minimum interfacial area would be achieved using the 14-faced cell, or tetrakaidecahedron, with six flat, square faces and eight hexagonal faces, slightly curved to accommodate Plateau's laws. In 1919, Desch [4] conducted the first survey of grain topologies in a polycrystalline metal. Instead of four- and six-edged faces, Desch found more pentagons than any other shape among the faces of 1000 brass grains. Weaire and Phelan [5] found a more efficient partitioning by reinterpreting Kelvin's constraint to allow a unit cell comprising eight polyhedra: six pentagonal dodecahedra (12 faces with five edges each) and two tetrakaidecahedra (14 faces: two with six edges and 12 with five edges each), wherein the pentagonal faces are slightly curved and the hexagonal faces are flat. In studies of soapy froths, metal grains and simulated polycrystals undergoing self-similar or "normal" grain growth, numerous authors have found similar frequency distributions of the number of edges per face [6–9]; each of these distributions has an average close to five edges. Kelvin's tetrakaidecahedron and the Weaire–Phelan cell are rarely observed. Glicksman [10] found the ideal

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solution for Kelvin's conjecture using abstract "average $\mathcal{N}$-hedra" (ANH) with identical faces, edges and vertices. Glicksman found the critical ANH, defined as that having zero Gaussian curvature in its faces, to have approximately 13.397 faces with 5.1 edges each; it cannot be constructed. This result can be interpreted as the extension ad infinitum of the Weaire–Phelan unit cell, taking the ensemble average of every face in a network of polyhedra [11].

Studying collapsing polycrystal grains, Steele [12] generated the Schlegel diagram [13] of almost every unique polyhedron with eight or fewer faces and mapped topologically valid transitions among them. This effort to enumerate the polyhedra in a metallurgical context was useful in identifying the available pathways to the tetrahedron, which must vanish due to its highly curved faces. The problem of enumerating all of the polyhedra is also of interest in mathematical circles, principally in analyzing the difficulty of doing so. In particular, the total number of unique convex polyhedra up to 15 faces have been determined by Federico [14], Duijvestijn [15] and Engel [16]. Partial graphical enumeration and calculation of the total number of unique 16-hedra was done by Voytekhovsky and Stepenshchikov [17]. Of the most direct relevance, Brinkmann and McKay [18] described an algorithm to enumerate the graphs of unique convex polyhedra for an arbitrary number of faces; they released its implementation as the open-source `plantri` software package. The total numbers of unique polyhedra with $4 \leqslant f \leqslant 20$ faces are summarized as the third column in Table 1. On our 3.3 GHz workstation, `plantri` enumerated each of the 57.9 billion unique icosahedra in 65 h.

Substantial efforts have been undertaken to systematically identify the topologies of grains present in polycrystals. To specify the topology of a given polyhedron, more information is needed than the number of edges belonging to each face. For example, the six tetragonal and eight hexagonal faces of Kelvin's tetrakaidecahedron can be rearranged to produce two more topologically distinct polyhedra. Rhines and Patterson [19] sketched Schlegel diagrams from stereoscopic observations of 500 aluminum grains after liquid gallium embrittlement and separation; these were used to analyze the frequency distribution of the numbers of faces per grain and edges per face. Recently, Patterson et al. [20] extended this work by analyzing the topology of each grain in Monte Carlo grain growth simulations and summarizing the frequency of observation associated with each Schlegel diagram for the unique convex polyhedra with $4 \leqslant f \leqslant 8$ faces. Patterson et al. enumerated a number of non-convex Schlegel diagrams, but one solitary grain with such a configuration was observed in all their datasets. In recent work, Lazar et al. [21] described a systematic approach to recording the topology of every grain in a polycrystalline dataset using Weinberg vectors [22] – that is, strings of letters or numbers encoding the connectivity of each vertex (or "corner") of the grain. The original grain topology can be reconstructed from this encoding, a significant improvement over the p-vector approach of Barnette [23] used previously [24]. Mason et al. [25] applied the fundamental concept of Weinberg vectors to vertices in networks of polyhedra in situ: rather than encoding the topology of a specific grain, Mason encodes the topology of every vertex in a "swatch" within a specific number of edges from a chosen root. The distribution of swatches generated from a microstructure can then be used to compute its topological distance from a reference microstructure, and to evaluate similarity in the topological makeup of different microstructures.

In this paper, we present our methodology for comparing the subset of grain topologies present in a microstructure to the domain of unique polyhedra. We apply this method to microstructures generated by various processes and discuss the differences in topologies expressed in each population. The processes and populations of interest are listed below on a subjective scale of "realism," from the

Table 1
Summary of enumeration progress for polyhedra with f faces using `plantri` and our Monte Carlo algorithm (partially enumerated classes are indicated in bold).

f	v	Total simple graphs	Enumerated simple graphs	Enumerated graphs with band-faces
4	4	1	1	0
5	6	1	1	0
6	8	2	2	1
7	10	5	5	3
8	12	14	14	15
9	14	50	50	**64**
10	16	233	233	**352**
11	18	1249	1249	**2096**
12	20	7595	7595	**14,011**
13	22	49,566	**49,565**	**98,119**
14	24	339,722	**327,848**	**376,266**
15	26	2,406,841	**605,124**	**426,414**
16	28	17,490,241	**413,265**	**219,886**
17	30	129,664,753	**113,213**	**53,713**
18	32	977,526,957	**81,311**	**19,241**
19	34	7,475,907,149	**67,029**	**7118**
20	36	57,896,349,553	**369**	**732**