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AVERAGE $\mathcal{N}$-HEDRA AS DESCRIPTORS OF 3-D NETWORK CELLS

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Summary Network cells represent physical entities, such as grains in polycrystals, bubbles in foam, or cells in biological tissues. We represent network cells with $\mathcal{N}$ neighbors by "proxies" called average $\mathcal{N}$-hedra, satisfying space filling and network topological averages. Analysis of the set of $\mathcal{N}$-hedra yields estimates of the metric and energetic properties of irregular cells in isotropic foams and polycrystals as functions of the number of neighbors, $\mathcal{N}$.

INTRODUCTION

The energetics and growth kinetics of space-filling networks, such as polycrystals and foams, remain important topics within the general subject of microstructure evolution. The foundation for grain and bubble growth in two dimensions was established a half-century ago by C.S. Smith [1] and J. von Neumann [2], and by W.W. Mullins [3]. This paper reports on an analysis of idealized "average $\mathcal{N}$-hedra" (ANH's) that may be used as "proxies" to determine the excess free energy and growth kinetics of an isotropic network structure in $\mathbb{R}^3$. ANH's have $\mathcal{N}$ identical curved faces, each enclosed by $p = 6 - \frac{12}{\mathcal{N}}$ edges; $2(\mathcal{N}-2)$ identical vertices equidistant from its centroid; and $3(\mathcal{N}-2)$ identical curved edges. ANH's form a complete set for $3 \leq \mathcal{N} \leq \infty$, although only four members ($\mathcal{N} = 3, 4, 6,$ and 12) are actually constructible, i.e., where p is an integer. All other ANH's are abstract geometric forms. Nonetheless, each ANH provides a descriptor of the average geometric, energetic, and kinetic properties of all irregular network cells within the same class, $\mathcal{N}$. Figure 1 compares an ANH with an irregular member of its class, $\mathcal{N} = 12$. Note that the ANH shown on the left has 12, identical, slightly bulging, pentagonal faces, whereas the irregular 12-hedron on the right contains a mixture of quadrilateral, pentagonal, and hexagonal faces. The p-value, vertex count, etc., according to Euler's theorem, are nonetheless identical.

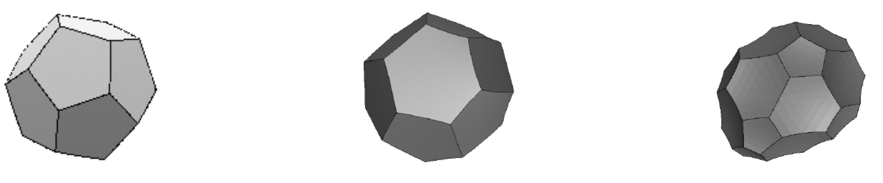

Figure 1. ***Left****: Average* 12*-hedron, consisting of identical pentagonal faces. Its* 20 *identical vertices are positioned equidistant from the volume centroid.* ***Middle****: Irregular* 12*-hedron exhibiting of a mixture of quadrilateral, pentagonal, and hexagonal faces. The* <u>*average*</u> *properties of any* 12*-hedron in an isotropic network (number of edges, vertices, p-value, vertex image, average dihedral angle, etc.) are identical to those of its ANH proxy.* ***Right****: Irregular* 24*-hedron, for which a constructible ANH does not exist. Note its concave faces. Renderings provided through the courtesy of Dr. S.J. Cox, Trinity College, Dublin, Ireland [4].*

NETWORKS IN 3-D

Geometry of ANH's

The area, $\mathbb{A}(\mathcal{N})$, and volume, $\mathbb{V}(\mathcal{N})$ of any ANH, are expressible as fractions of the corresponding areas and volumes of a sphere with the same radius of curvature as that of the faces of the ANH. These are, respectively,

$$\mathbb{A}(\mathcal{N}) = \mathcal{G} \cdot A_{sph}, \quad \text{and} \quad \mathbb{V}(\mathcal{N}) = \mathcal{F} \cdot V_{sph}, \tag{1}$$

where the fractions $\mathcal{G} = \frac{1}{4\pi}\iint_{faces} K dA$ is the ratio of the total spherical image of the ANH to that of a sphere (4π), and $\mathcal{F} = \frac{\mathcal{N}}{2} + \frac{\mathcal{N}-2}{16\pi}\left[2^{\frac{3}{2}} - 57 \arccos\frac{1}{3} + 33 \arcsin\left(\frac{2}{\sqrt{3}}\cos\frac{\pi}{p}\right) - \tan\arcsin\left(\frac{2}{\sqrt{3}}\cos\frac{\pi}{p}\right)\right]$. The integral of the Gaussian curvature, K, appearing in the area fraction, $\mathcal{G}$, can also be found exactly for any ANH using the Gauss-Bonnet theorem,

$$\iint_{faces} K dA = 4\pi - 3(\mathcal{N}-2)\Omega^{edge} - 2(\mathcal{N}-2)\bar{\Omega}, \tag{2}$$

where the constant $\bar{\Omega} = 0.551287\ldots$ is the spherical image of each trihedral vertex as demanded by topology. The function Ω^{edge} is the spherical image contributed by each curved edge and varies with $\mathcal{N}$ according to the formula

$$\Omega^{edge} = \pi + 2\arctan\left(\sin\frac{\alpha(\mathcal{N})}{2}\tan\frac{\pi}{p}\right) - 2\arccos\left(-\frac{1}{3}\right), \tag{3}$$

where $\alpha(\mathcal{N})$ is the angle between poles located on an ANH at the geometric centers of adjacent faces, namely

$$\alpha(\mathcal{N}) = 4\arctan\sqrt{1 - 2\sec\left(\frac{\pi}{2(\mathcal{N}-2)}\right)\cos\left(\frac{\pi(2\mathcal{N}-3)}{6(\mathcal{N}-2)}\right)}. \tag{4}$$

Network energetics

The excess free energy of a 3-d network, ΔF, such as a foam or polycrystal, is given by its interfacial area sum

$$\Delta F = \frac{\gamma}{2}\sum_i A_i = \frac{\gamma}{2}\sum_i e(\mathcal{N}_i)\,[V(\mathcal{N}_i)]^{\frac{2}{3}}, \tag{5}$$

where γ is the specific interfacial free energy of the faces of the polyhedra. Cox and Fortes [5] showed that the free energy, may be expressed as a sum over the volumes of polyhedral network cells as shown in the second equality displayed in Eq.(5), where the dimensionless ratio, $e(\mathcal{N})$, is defined as

$$e(\mathcal{N}) \equiv \frac{\mathbb{A}(\mathcal{N})}{[\mathbb{V}(\mathcal{N})]^{\frac{2}{3}}}. \tag{6}$$

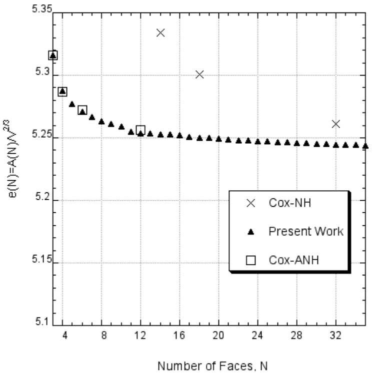

Figure 2. *Plot of $e(\mathcal{N})$ versus $\mathcal{N}$. Shown are the analytical values derived here for ANH's (solid symbols), and recent simulation data reported by Cox and Fortes for constructible ANH's (open squares) and irregular network $\mathcal{N}$-hedra (crosses) [5].*

Equation (6), which is scale independent, is easily evaluated with the analytical expressions for the areas, $\mathbb{A}(\mathcal{N})$, and the volumes, $\mathbb{V}(\mathcal{N})$, shown in Eqs.(1). Cox and Fortes [5] extended results derived originally by Vaz et al. for 2-d networks [6], and confirmed that in 3-d the ratio $e(\mathcal{N})$ also varies extremely weakly with $\mathcal{N}$. Figure 2 provides a comparison of the present analytic results, as expressed through Eq.(6), with the numerically computed values reported by Cox and Fortes for several $\mathcal{N}$-hedra using Brakke's surface evolver [7] to evaluate the areas and volume. The analytical values for $e(\mathcal{N})$ agree well with the values computed by Cox and Fortes, especially in the four cases where the simulated $\mathcal{N}$-hedra correspond to constructible ANH's ($\mathcal{N} = 3, 4, 6,$ and 12). For the three cases reported in [5] where the polyhedra are not ANH's, the simulations yield slightly higher values (0.5% to 2%).

Coxeter [8], and more recently, DeHoff [9] showed that the average number of faces per polyhedron in a large isotropic 3-d network is $\langle\mathcal{N}\rangle \approx 13.397$, corresponding to the "ideal" flat-faced cell that satisfies local equilibrium. The average value $\bar{e} \approx 5.254$, so after substitution into Eq.(5) the total excess free energy arising from its interfaces of an isotropic 3-d network consisting of i polyhedral cells is

$$\Delta F \approx 2.63\,\gamma \sum_i [\mathbb{V}(\mathcal{N}_i)]^{\frac{2}{3}}\,. \tag{7}$$

CONCLUSION

Highly symmetric average $\mathcal{N}$-hedra (ANH's) may be used as topological "proxies," or descriptors for polyhedral network cells. Although ANH's are constructible only in a few cases ($\mathcal{N} = 3, 4, 6, 12$), their general analysis yields important geometric and energetic properties of *all* irregular (constructible) network cells. The kinetic properties of ANH's and the evolution of 3-d network structures will be discussed elsewhere [10] due to space limitations.

References

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