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***Materials Science***

# Mathematics and Polycrystalline Materials: An Entropic Approach to Texture Development

*By Richard Sharp*

Metals and ceramics are polycrystalline materials, solids formed from a dense network of grains (Figure 1). Function follows form for these materials: The properties of the network affect the mechanical, electrical, thermal, and other properties of a sample. In a metal like copper, the grains are chemically identical, and it is crystallographic orientation that distinguishes neighboring grains. Grain boundaries are dynamic, driven by an interfacial energy that causes some grains to shrink and vanish, others to grow. The result is a general coarsening process that is fertile ground for mathematicians as well as materials scientists.

Grain networks received significant attention at this year's SIAM Conference on Mathematical Aspects of Materials Science (see the article by Selim Esedoḡlu). Indeed, the importance of treating polycrystalline materials as an interactive network rather than a collection of individual grains was the premise of a presentation by Christopher Shuh. Network dynamics, in particular mesoscopic PDE models based on front tracking, was a frequent topic. Both for two-dimensional thin films and in three dimensions, such models prescribe that the normal velocity of an interface is proportional to its mean curvature, the interfacial energy, and mobility, a physical parameter. A natural energy-minimizing boundary condition, the Herring condition, determines the geometry of triple junctions, the stable intersection of three grains. The result is a large dissipative system of mesoscopic PDEs in which energy is the integral of the interfacial energy over all boundaries in the network [3].

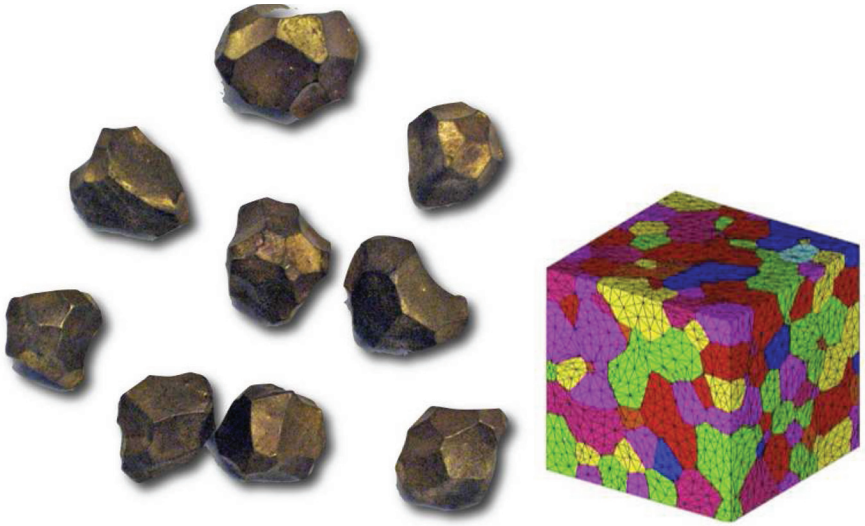

**Figure 1.** *Grains and grain networks: Beta brass grains (left) and visualization of a meshed grain network (right).*

A range of numerical methods are available for simulating such systems; a number of them were presented at the conference, including implicit methods (by Esedoḡlu, Elsey, and Smereka [2] and independently by Wilson and Rollett); explicit methods (by Ta'asan [3]); a dislocation-based approach (by Srolovitz [5]); and grain network simulation via proxy, using closely packed colloids (by Frans Spaepen). Stable statistics of evolving grain networks were a common theme of the simulations: The distribution of grains by number of sides and the normalized distribution of grain size, for example, are robust statistics across a wide range of parameters and initial configurations. An intriguing property, texture as measured by the grain boundary character distribution (GBCD), is characteristic as well as robust [4]. Simulation reveals that high-energy boundaries are quickly eliminated and, strikingly, that GBCD adopts a Boltzmann-like profile, dependent on the material-specific interfacial energy (Figure 2). A theory for the GBCD was the main topic of Epshteyn's talk.

GBCD is the distribution of boundaries (weighted by length in two dimensions, by area in three) with respect to interfacial energy. At the conference Epshteyn presented a theory for the development of GBCD in the context of a simplified critical-event model and Emelianenko gave a detailed introduction to the simplified model. Barmak, Eggeling, Emelianenko, Epshteyn, Kinderlehrer, Sharp, and Ta'asan [1] are investigating the topic as part of a collaborative effort.

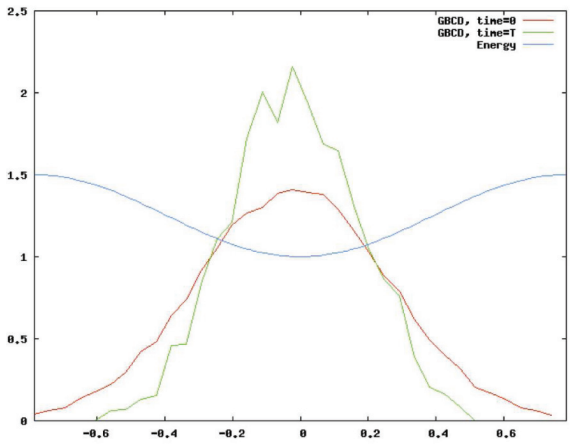


**Figure 2.** *GBCD evolution with energy* $\psi(\alpha) = 1 + \varepsilon(\sin 2\alpha)^2, -\frac{\pi}{4} \leqq \alpha \leqq \frac{\pi}{4}, \varepsilon = 1/2.$

A network is formed by a random partition of the unit circle, where the subintervals are identified as grain boundaries with length $L_i$ (the subintervals are not "one-dimensional grains") and a randomly assigned orientation $\alpha_i$. Each boundary contributes $L_i\psi(\alpha_i)$ to the total energy of the system, where $\psi(\alpha)$ is a given function describing the interfacial energy. The dynamics of the boundaries are determined by gradient flow. A critical event occurs when a boundary reaches zero length: It is removed and its former neighbors are connected. The network dynamics are dissipative between critical events.

The energy conservation relation between critical events and Young's law lead to an energy inequality satisfied by the system in terms of $\Sigma_i (dL_i/dt)^2$. A key observation is that this inequality can now be translated into a statement about GBCD: $\rho(\alpha,t)$. This is done by identifying $\rho$ as the length-weighted histogram of segments over $\alpha \in \Omega$. Now comes the crucial step: addition of an effective entropy. Memoryless critical events have produced an irreversible system, for which distributional dynamics are sought. Though

not the only choice, adding the standard configurational entropy leads to a dissipation relation involving the Wasserstein metric. It forms the basis for a Wasserstein metric implicit scheme consistent with solutions to the Fokker–Planck equation,

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial \alpha}\left( \sigma \frac{\partial \rho}{\partial \alpha} + \frac{d\psi}{d\alpha}\rho \right).$$

The dissipative behavior of GBCD thus reveals an underlying Fokker–Planck form.

The value of the parameter $\sigma$ is not known a priori, but is revealed through simulation by finding the value that causes the Kullback–Leibler relative entropy to vanish as $t \to \infty$,

$$\sigma = \lambda \text{ such that } \Phi_\lambda(\rho) = \int_\Omega \rho \ln\left[\frac{\rho}{\rho_\lambda}\right] d\alpha \to 0,$$

where $\rho_\lambda$ is the stationary Boltzmann distribution of the Fokker–Planck equation with parameter $\lambda$ (Figure 3, left). The result is an entropic theory for the development of GBCD and a program for discovering the system's effective "temperature." Numerical experiments have revealed high-quality predictions for GBCD, as shown in Figure 3, right.

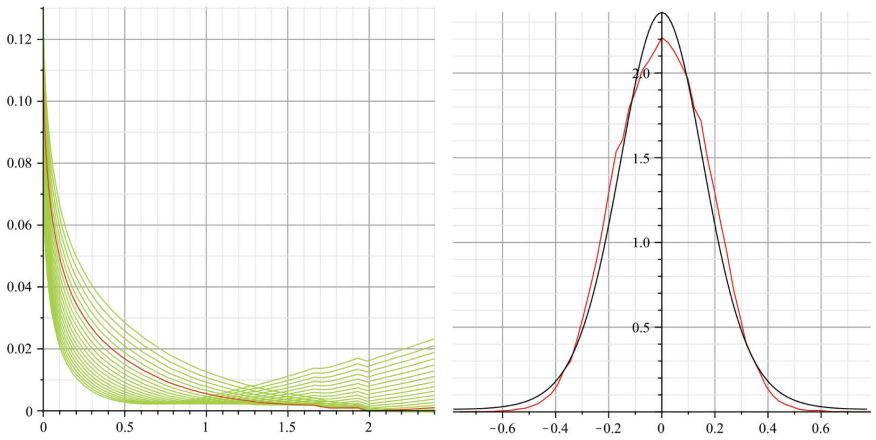


**Figure 3.** *Relative entropy determines $\sigma$. Left: Relative entropy as a function of time for various $\sigma$. Right: GBCD and the Boltzmann distribution when $\sigma = \lambda$.*

## References


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