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Topological changes in coarsening networks

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ABSTRACT

Curvature driven grain growth proceeds by the motion of curved grain boundaries in polycrystals leading to a decrease in the total interfacial free energy. However, grain growth cannot occur without the so-called topological transitions. Indeed, it is a mathematical impossibility that a decrease in the number of grains per unit volume may take place without the topological transition that corresponds to the grain disappearance. Nonetheless, despite their importance, no previous work has studied the topological transitions in detail that take place during the transient as well as the self-similar state of coarsening. In the present work, the three classical topological changes are tracked during 2-d grain growth simulated by a Monte Carlo method. It is shown and discussed how topological transitions reach a self-similar state together with the grain size and the number of edges (faces) per grain distribution.

1. Introduction

The geometric topology of polygonal networks in materials like grain and foam microstructures has been a topic of scientific interest for decades—not only for mathematicians but also for materials scientists. Such networks consist in two dimensions of edges and vertices. As a result, a certain number of edges and likewise vertices surround a polygonal area—a cell or a grain.

Particularly, the question of coarsening of such systems is of great importance since the mechanical properties of most materials depend on their microstructures. Ideal coarsening is a process, where it is assumed that all edges are characterized by the same energy per unit length and by the same mobility. Three edges meet in a vertex, the dihedral angles must be 120° and so the edges connecting two neighboring vertices are usually curved. From a thermodynamic point of view, this state is not in equilibrium. The curved edges have an excess energy that the network reduces during coarsening. Consequently, the boundaries move to the center of curvature reducing the edge length, but at the same time opening a contest between the motion of the edges and the equilibrium dihedral angles. This process results in a coarsening of the network, where small (convex) cells shrink and at some point, disappear, while large (concave) cells grow increasing the average cell size.

A well-investigated example for ideal coarsening is normal grain growth of polycrystalline metals or alloys on the micrometer scale, which has been explored by experimental, computational, and theoretical means (compare, e.g., [1–7]). It is known that in case of normal grain growth the average linear grain size of an ensemble of polycrystalline grains fulfills a square-root law regarding the coarsening time in two as well as in three dimensions. At the same time, the network is in what is called a quasi-stationary state showing statistical self-similarity. The latter can be analyzed for instance by observations of the scaled grain or cell size distribution as well as the relation between number of edges and relative grain size. Both analyses yield time-independent results, and self-similar scaling is a well-accepted property for ideal coarsening.

Specifically, topological considerations of such polygonal networks have been of immense significance, e.g., for mean-field theories of grain growth. In his classical theory of grain growth, Hillert [8] originally neglected any topology-size-relationship. The resulting grain size distribution function has never been observed, neither in experiments nor in computer simulations. However, taking such relations between neighboring cells into account has advanced the analytic theories such that nowadays the resulting size distribution functions are self-similar, show volume conservation, and are suitable for fitting measured experimental and simulated size distributions (e.g., [9–11]).

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Nevertheless, a number of questions still remains to be answered—even today. One of those is the question regarding the occurrence of topological changes in the coarsening networks. As we have seen above during coarsening the edges move and small grains shrink and disappear. These are, of course, not detached events, but happen within the network, where a moving edge is always dragging its vertices along and therewith also the connected edges in the vertices making it a complex, competing motion. Nevertheless, from a purely topological point of view the number of events changing the local topology is very limited:

1. It is possible to change the local topology, while keeping the total number of edges and vertices in the network constant. This is done by a neighbor switching event, T1, as shown in Fig. 1a, where the edge between two neighboring cells vanishes disconnecting them but making at the same time a new connection between two further neighboring cells.
2. During an edge disappearance event, T2, a cell is losing one edge and the two adjacent vertices merge, which can be seen in Fig. 1b. As a result, in that moment, where the boundary is annihilated, four boundaries meet in a vertex, which is highly unstable, and hence the local topology has to readjust.
3. Finally, a whole grain can vanish during a grain disappearance event, T3, merging here also the connected vertices. This event usually happens with three-sided cells removing three edges and two vertices as in Fig. 1c, but could possibly also occur for small four-sided grains resulting just for a moment in an unstable quadruple junction.

All in all, we can see in Fig. 1 that such topological events are often accompanied by a reduction in the number of edges and neighboring cells, respectively—a point that we will discuss below.

Of course, the general topic of topological changes in cellular networks has been in the center of attention of materials scientist for many years:

Already more than 40 years ago, Rhines et al. [12] pointed out that "Topological transformations simply happen when the Euclidean dimensions of some part of the system chance to pass through zero. This occurs when a grain goes to zero volume and when a triangular face goes to zero area, or is created. Such events can occur only as grain boundary sweeps through the system."

In more recent times, Wakai et al. [13] analyzed topological transformations of grains in 3D normal grain growth using the Surface Evolver method. They focused on grain switching and grain disappearance events and found that individual grains increase and also decrease their number of faces many times as the grains grow or shrink, where the reduction in the number of faces happens more often than the generation of new faces.

In a more recent paper, Sprague et al. [14] distinguished for two-dimensional grain growth three types of topological events: loss of the simplest grains (type I event), grains gaining one edge (type II event), and grains losing an edge (type III event). These are clearly different from our above defined events T1 to T3. Nevertheless, they already found a constant ratio of the number fraction of disappearing grains to the area fraction swept by the grain boundary as well as a constant ratio of boundary-switching events per grain disappearance.

In addition, the topic of topological changes is often a very important focal point of investigations of coarsening using the vertex model. For example, Weygand et al. [15] used vertex models for the simulation of grain growth and investigated the problem of the implementation of topological transitions in the model, which is based on the introduction of virtual vertices. Also Barrales-Mora et al. [16] used the vertex model commenting on the implementation of topological changes in their model. But they mention in particular that in their case the "rate of change … is less affected by the change of the topological class than by the change of the metrics of the grains".

In the following, we analyze the three types of topological changes occurring in two-dimensional polygonal networks. To that aim, Potts model simulations of ideal coarsening have been carried out for different initial networks and at different coarsening stages. We will follow the temporal development of the topological changes as well as the trajectories of individual cells.

2. Topological events during self-similar coarsening

In the present work, we have employed the lattice-based Monte Carlo Potts model for ideal coarsening assuming that there are only two parameters characterizing the material—namely the parameter γ in the Hamiltonian of the simulation algorithm measuring the energy interaction of a lattice point with all neighboring lattice points, which is related to the specific edge energy of the network, and the parameter m in the transition probability describing the specific edge mobility of the network. The vertices are considered to be part of the edges and have, therefore, no direct influence themselves. For a detailed description of the Potts model please compare, e.g., [17,18].

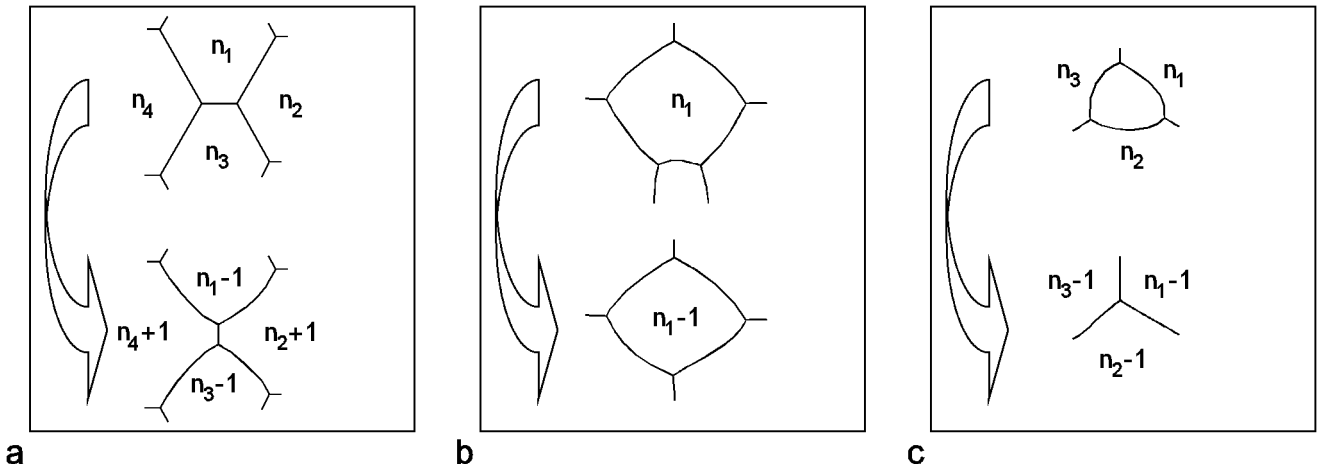

Fig. 1. Three types of topological changes occurring in two-dimensional networks: a – neighbor switching events T1; b – edge disappearance events T2; c – grain disappearance events T3.