APPLICATIONS OF MICROSTRUCTURAL MODELING

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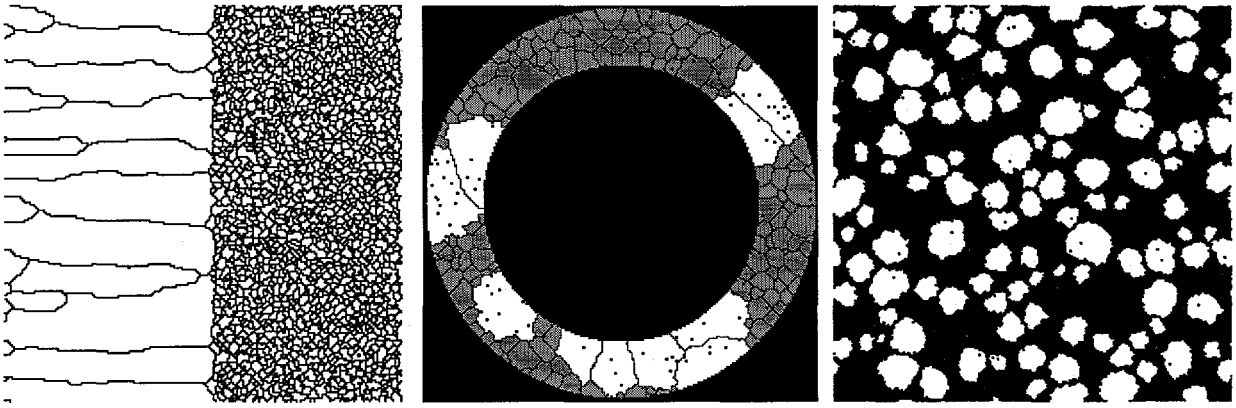
Detailed and rigorous computer simulations of microstructural evolution have been developed over the past decade. Although models differ widely, all methods share the characteristic of resolving structural details on a microstructural level and following evolution of structure on a realistic time scale. We can loosely divide simulation methods into boundary models and bulk models.

Boundary models map the microstructure in terms of the internal interfaces present in the system. In vertex models, the motion of interface junctions controls evolution; junction motion is driven by line tension from the attached interfaces [1]. In surface models, the motion of internal interfaces is modeled directly. Each portion of an interface moves toward its center of curvature, then angular boundary conditions at interface junctions are adjusted accordingly [2].

Bulk models map the microstructure by discretizing or bitmapping the structure. Evolution involves changing the characteristics of the elements or pixels in the structure. In spin models, each element is assigned to a particular grain, and internal interfaces occur when unlike elements are neighbors. Evolution occurs by changing or swapping the characteristics of particular elements according to energetic rules [3]. In diffuse models, elements belong proportionally to the grains in the system, and a continuum energy minimization technique drives motion of the diffuse interfaces in the system [4].



(a) (b) (c)

Figure 1. Examples of computer simulated microstructures and evolution processes. (a) Zone annealing of a fine-grained polycrystal. The sample is pulled through the hot zone from right to left. The hot zone position is at the center of the sample, and the right hand side of the sample is unannealed [10]. (b) Recrystallization in a toroidal wire containing a dispersion of inert particles. Gray grains are unrecrystallized and white grains are recrystallized. (c) Grain structure due to Ostwald ripening of solid grains in a continuous liquid matrix [8].

Each simulation type has been successful in modeling the single phase, isotropic grain growth problem. Boundary models have the advantage of simulating geometric, sharp internal interfaces and junctions. They are especially appropriate for problems in which interface and

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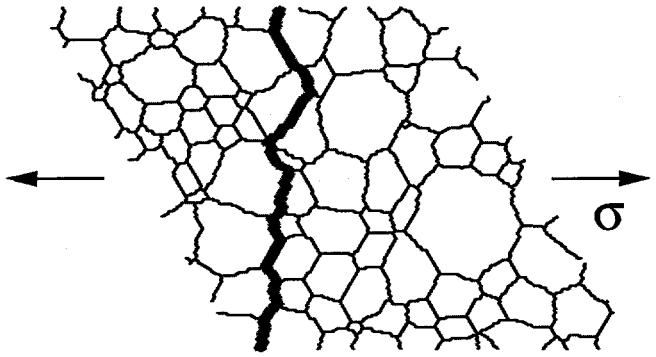
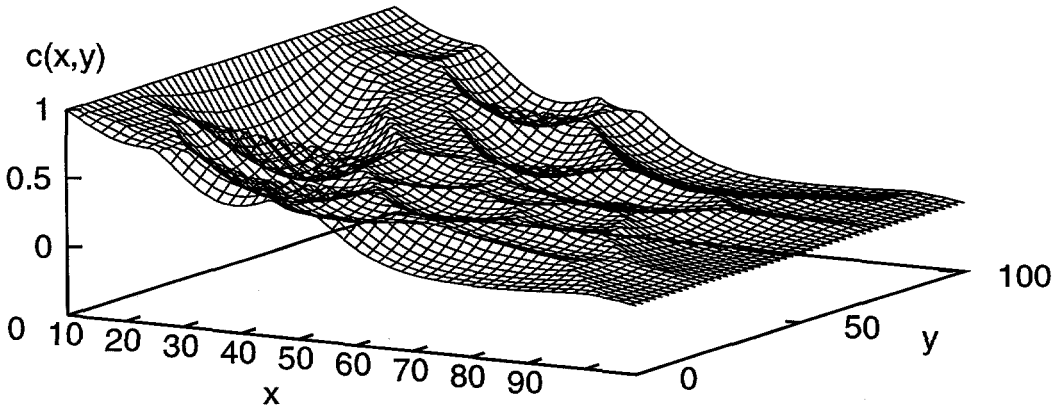
surface properties govern evolution of structure. Surface models have been extended to three dimensions, although to date vertex models are still strictly two-dimensional. Boundary models have been used successfully to model grain boundary grooving [2], abnormal grain growth and the effects of free surfaces on growth in films [5]. Bulk models are able to more easily include bulk driving forces and long-range diffusion processes. They are extendible to three dimensions, and have been successfully utilized for problems such as recrystallization [6], sintering [7], Ostwald ripening [8], and solidification [9].

The first contribution of microstructural evolution simulations is in understanding complex evolution phenomena. Three examples, all generated by variations on the bulk Monte Carlo Potts model for evolution, are shown in figure 1. In figure 1(a), a fine-grained sample is being pulled through a hot zone. The grain boundary mobility varies with local temperature, and all other bulk and boundary properties are isotropic. Simulations predict which pull speeds allow the columnar structure in figure 1(a) to form [10]. In figure 1(b), recrystallization is occurring in a toroidal wire containing a dispersion of inert particles. Simulations show the strong dependence of recrystallized grain structure on nucleation conditions. Figure 1(c) shows a grain structure which has evolved via Ostwald ripening of solid grains in a continuous liquid matrix. Simulations have reproduced grain size distributions in good agreement with experimental data.



(a)



(b)

Figure 2. Examples of computer simulated microstructures used to understand material properties. (a) Crack propagation in a brittle polycrystal. The thick line shows the minimum energy intergranular crack path starting from a notch and extending across the sample. (b) Solute diffusion through a polycrystal with high diffusivity grain boundaries. Solute concentration is held at unity at x = 0 and at zero at x = 100 [11].

The logical extension of microstructural evolution simulations is to use the structures and other data generated to understand materials properties and performance. This is certainly the area that represents the greatest challenge and largest potential payoff for the next decade of microstructural modeling. Two examples of using simulated microstructures to understand materials properties are shown in figure 2. Figure 2(a) shows a minimum energy intergranular crack path starting from a notch and extending across an equiaxed polycrystal. The crack model used is quite simplistic; there is a need to develop better linkage between microstructure and mechanics simulations. In figure 2(b), one edge of a two-dimensional grain structure is held at a solute concentration of unity. A finite difference algorithm generates the solute concentration profile during transient state solute diffusion. Peaks in the profile clearly show fast-transport grain boundaries, and large grains show deep concentration valleys [11].

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