Commentary

Mathematically Modeling Mesoscale Microstructural Evolution

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Many microstructural changes that occur in materials can be explained using simple physical models. For example, we know that boundaries or interfaces have higher energies than grain interiors and as the size of an object increases, the surface area-to-volume ratio decreases. Therefore, it is easy to understand that grain growth or coarsening of a precipitate takes place because the material is minimizing the overall grain or interfacial boundary energy as the grain or phase size increases. Furthermore, simple kinetic models can be developed to explain how the grain size or phase size changes with time by considering the rate of boundary or interface motion.

Accordingly, mathematical models of microstructural evolution can often be derived based on the underlying physics. In principle, by numerically solving the mathematical equations and taking into account appropriate boundary conditions, the microstructural evolution of a system can be modeled on a computer. In reality, it is extremely difficult to do so using such a straightforward approach since all of the interfaces during a microstructural evolution are moving. Therefore, there has been enormous effort both in the materials science and applied mathematics communities to develop innovative mathematical models for predicting the temporal and spatial microstructural evolution.

The first nontraditional model, the Monte-Carlo Potts model for grain growth, was developed more than ten years ago. This model avoids the explicit tracking of moving interfaces, yet captures the essential physics that the interfaces move to reduce the total interfacial energy.[1,2] Since then, there have been many advances in the mathematical modeling of microstructural evolution, particularly in the last five years. For example, about 70 papers were presented at Materials Week '95 by mathematicians and material scientists on models for predicting microstructural evolution during phase transformations, grain growth, coarsening, effect of elastic stress, and other related topics.[3]

In this issue of *JOM*, the following articles describe nontraditional mathematical models for modeling microstructural evolution. In the first article, Chen and Wang overview a method in which a diffuse-interface field model is used to predict microstructural evolution. In contrast to models that employ a conventional sharp interface to describe the boundary between grains or phases, the field model utilizes a set of field variables that are functions of spatial coordinates. They describe how the microstructures can be described by a set of spatially dependent field variables, how to incorporate different thermodynamic driving forces for microstructural evolution, and the evolution equations, then describe several applications of this approach.

In the second article, Taylor discusses how mathematical models based on surface curvature can be used to describe thermodynamic driving forces for modeling interface growth and shape changes. She discusses the concepts of mean curvature, which is appropriate for isotropic surface free energy, and weighted mean curvature, which is appropriate for anisotropic surface free energy. The latter is extended to include anisotropic surfaces that are faceted, and, although not discussed in this article, it has been shown recently that in solving problems in which crystals are fully faceted, this anisotropy makes problems more easily solvable than for lesser anisotropies.[4] Finally, she briefly presents several examples in which these models can be used to examine the evolution of two-dimensional shapes controlled by surface diffusion and surface-attachment limited kinetics.

Are these types of mathematical models merely computer toys or they are of interest to engineers in the materials field? Consider a specific problem:

> The stress-induced directional coarsening of γ' precipitates in nickel-based superalloys has been observed in high-volume fraction single-crystal alloys and was first reported in 1967. The stress-induced coarsening produces a microstructure consisting of alternating lamellae of γ and γ', a so-called rafted microstructure. Experimental work has demonstrated that several parameters can influence both the morphology of the precipitates and the kinetics of the process—the difference (misfit) between the lattice parameters and the elastic constants of the γ and γ' phases as well as the sign and magnitude of the applied stress.[5] More recently, the role of dislocations generated during creep on the raft development has also been addressed.[6] If a complete mathematical description of all of these effects on the directional coarsening of γ' could be developed, it should then be possible to make predictions from computer simulations as to what effect changes in composition, phase-volume fraction, stress state, and magnitude would have on the directional coarsening behavior. That is, rather than going into the laboratory and producing a number of compositions and measuring the effect these changes in composition or stress states have on directional coarsening, the simulations should allow one to focus on the critical compositions to test the models.

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Are we there yet? Almost. As a matter of fact, the diffuse-interface field model discussed by Chen and Wang has been applied to this problem and is able to predict the effect of various factors, including composition, volume fractions, the lattice mismatch, the elastic inhomogeneity, and the sign and magnitude of the applied load.[7]

To effectively apply the existing models to actual materials design and determine which model to use in a given materials design will require much needed communication between materials designers and modelers. On one hand, designers will pose practical design problems and specify the kinds of information that can be used in the materials design. On the other hand, modelers should inform the designers of the sophisticated mathematical models that are available today or being developed. The time for communication between designers and modelers is now and not five or ten years down the road.

References

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