

Mesoscale Modeling of Stressed Grain Growth

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ABSTRACT

The microstructure of materials, i.e. the size, shape and arrangement of grains, determines essentially the material properties such as mechanical strength, toughness, electrical conductivity and magnetic susceptibility. In general the desirable property of materials can be controlled and improved by understanding of microstructure evolution processes in grain growth controlled by grain boundary migration, and grain boundary diffusion. The process of grain growth involves moving interfaces and topological changes of grain boundary geometry, and this cannot be effectively modeled by the Lagrangian, Eulerian, or Arbitrary Lagrangian Eulerian finite element method when stress effect is considered. In this work, we first introduce a variational equation based on the balance of energies associated with grain boundary surface tension and curvature, elastic strain energy, and the elastic strain energy difference due to anisotropy between adjacent grains. This reflects the coupling of elastic deformation of grains with grain boundary migration and thus necessitates the discretization of grain boundaries and grain domains. Using finite element method to study the migration of grain boundaries leads to a severe mesh distortion in each grain, and the topological changes of grain structures further demand a complete remeshing. To address these issues, a double-grid method is introduced. The elastic deformation of grains is discretized by a meshfree reproducing kernel approximation with built-in strain discontinuities along the grain boundaries, whereas the grain boundary migration kinematics is discretized using the standard finite element approximation.

NUMERICAL RESULTS

