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Using Kinetic Monte Carlo to Simulate Dendritic Growth

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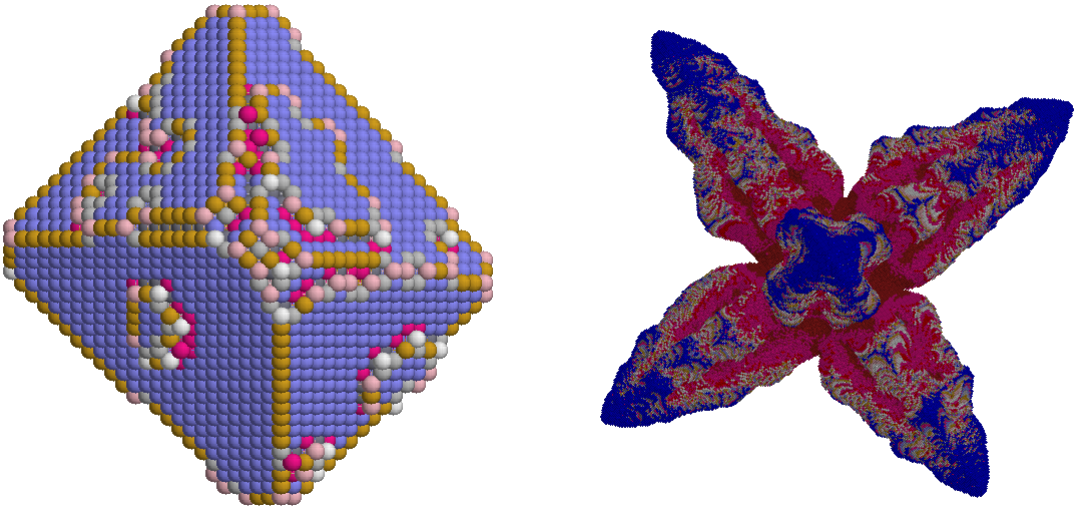
ABSTRACT

We consider a kinetic Monte Carlo approach to tracking the interface during the growth of a dendrite into an undercooled melt. For pure materials, morphological instability leading to dendritic growth is the result of interfacial perturbations growing into an environment that is below the material's melting temperature. This enhances the subsequent growth of the perturbations and eventually leads to an intricate, snow-flake like growth pattern. This is now a classical problem in computational science, but is normally studied with continuum models. On scales ranging from nanometers up to several microns, we aim to achieve atomistic resolution by augmenting standard KMC models for crystal evolution with a model for solidification that "deposits" atoms onto the growing crystal at an environment dependent solidification rate. As dendrites grow beyond the limits one can handle with KMC alone, one can imagine feeding the results into a continuum simulation as initial conditions. There are a number of computational advantages to this approach: effects due to fluctuations, which are important at small scales, are naturally included; the finite size of atoms is properly accounted for; and anisotropy requires no additional modeling beyond the choice of crystal lattice.

Within the bulk liquid and solid region, we solve the heat equation on a lattice that is commensurate with an FCC crystal lattice on which the crystal is forced to grow. As in the sharp-interface formulation of these models, the computational domain $\Omega \subset \mathbb{R}^3$ is decomposed into an inner, solid region Ω_S and an outer, liquid region Ω_L, separated by a closed surface Γ_I. The principal governing equation is the heat equation, with the Gibbs-Thompson equation determining the temperature on the interface. The position of the interface is determined via a stochastic model, which includes surface diffusion of the solid material and phase change at a rate proportional to the local undercooling. The growth of the interface occurs one atom at a time, with updates to the surrounding thermal field occurring on a coarser time scale. The free-boundary tracking has negligible computational cost compared to the tracking the thermal field, but does have significant memory requirements.



Results from a KMC model for growth of a dendrite into an undercooled melt. a) Early stages of growth ($\approx 10,000$ atoms, expanded to fill page) when the crystal is faceted. b) later stages of growth ($\approx 1,000,000$ atoms) revealing some key characteristics of dendrites. The shading/color indicates coordination number in figure (a) and temperature gradient in figure (b).