Direct handling of sharp interfacial energy for microstructural evolution

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We introduce a simplification to the previously demonstrated hybrid Potts–phase field (hPPF), which relates interfacial energies to microstructural sharp interfaces. The model defines interfacial energy by a Potts-like discrete interface approach of counting unlike neighbors, which we use to compute local curvature. The model is compared to the hPPF by studying interfacial characteristics and grain growth behavior. The two models give virtually identical results, while the new model allows the simulator more direct control of interfacial energy.
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Many microstructural evolution processes have been simulated by the Cahn–Hilliard (CH) equation based on the phase field model. The Cahn–Hilliard equation was originally developed to model spinodal decomposition [1] of glass with interfacial energy introduced by a gradient in the composition of the glass. Since then, many have adapted this to simulate a wide range of microstructural evolution mechanisms, with "order parameters" introduced by Khachaturyan [2] to represent many other materials characteristics, such as grains and precipitates, with gradients in the parameters representing interfaces. Recently, Homer et al. [3–5] introduced a hybrid Potts–phase field (hPPF) model, which uses both the CH smoothly varying interfacial energy and the Potts sharp interfacial energy terms to calculate the interfacial energy. In this work, we show that the CH–interfacial energy term can be eliminated; we can determine the interfacial energy of sharp interfaces between discrete particle and the bulk free energy by the compositional field. We will compare our results to those of the hPPF model, which has been extensively studied. The benefit of such a model is that it affords direct control over the thermodynamics of interfaces.

These interfaces between microstructural features are sharp interfaces with the associated interfacial energy, γS, and the bulk energy is a function of phase and composition.

Several types of computational techniques have been used to model the evolution of microstructures, e.g. Potts Monte Carlo (PMC) and phase field (PF) models. The former uses a discretized ensemble of particles, while the latter uses continuum fields, or order parameters, to define the microstructure. PMC has sharp interfaces with discretized curvature where digitized microstructural features are used to calculate the interfacial energies. In contrast, PF models use the CH equation [1,6–8], where the interfacial energy is a function of the gradients in the continuous fields. While these models have been extensively used for different types of microstructural evolution, both have intrinsic drawbacks. The PMC model struggles to simulate smoothly varying continuous fields, like concentrations, while the PF model requires a large set of coupled partial differential equations with meshes sufficiently refined to accurately capture diffuse interface evolution. These issues can easily become prohibitively computationally expensive. Therefore, Homer et al. developed the hPPF model, which enables efficient and accurate simulation of microstructural evolution, where microstructures

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Table 1. Numerical values of the model's parameterization variables used in the presented simulations.

Parameterization variable	C_1	C_2	C_3	C_4	λ_0	λ_1
Values	0.25	0.75	0.05	0.95	0.3	0.5

are characterized by both continuous fields and discrete particles, and the total interfacial energy is the sum of both CH and the PMC interfacial energies. We show that the hPPF can be further simplified to only consider the PMC interfacial energy.

Our model runs in a digitized voxeled mesh with a continuum concentration field overlaid on it. The voxels are populated by an ensemble representing the different microstructural features. The microstructure is represented by a set of discrete fields, grain id (s) and phase (q), and a continuum field, concentration (C). The concentration, $C \in \mathbb{R} : 0 \leqslant C \leqslant 1$, defines the fraction of component B at a point in the continuum field. The grain id and phase are integer discrete values that denote the membership of that voxel in a particular grain and its phase, respectively. For the grain growth simulation, we have a two-phase binary system where each phase is allowed a set of grain ids.

The thermodynamic state of the system is given by an equation of state (EoS), which has volumetric and interfacial terms. The hPPF model uses a free energy functional that incorporates the gradient in composition term used by the CH equation and the Potts term, i.e. total number of dissimilar neighboring voxels,

$$F = \int_{\mathcal{V}} f_0 dV + \int_{\mathcal{S}} \gamma dS$$
$$= \int_{\mathcal{V}} f_0 dV + \frac{\gamma_{CH}}{2} \int_{\mathcal{V}} |\nabla C|^2 dV + \gamma_{Potts} \int_{\mathcal{S}} dS \quad (1)$$

where f_0 is the bulk chemical free energy and the γs are the interfacial or surface energy. The CH term goes to zero as we move away from the interface,

$$\lim_{d_{int} \to \infty} \nabla C = 0 \quad (2)$$

where d_{int} is the distance to the sharp interface. Our model only uses the Potts term to account for the interfacial energy induced by the curved surface (curvature), which gives us

$$F = \int_{\mathcal{V}} f_0 dV + \gamma_{Potts} \int_{\mathcal{S}} dS \quad (3)$$

We use polynomial (quadratic) equations to describe the bulk chemical free energies

$$f = \int f_0 dV = \sum_{i=1}^{N} f_i(q_i) \quad (4)$$

where N is the total number of sites (voxels) in the simulation system and each site i with q phase stores energy

$$f_i = \begin{cases} \lambda_0 \left[(C - C_1)^2 + (C - C_2)^2 \right] + \lambda_1 (C - C_3)^2, & q = \alpha \\ \lambda_0 \left[(C - C_1)^2 + (C - C_2)^2 \right] + \lambda_1 (C - C_4)^2, & q = \beta \end{cases} \quad (5)$$

where f_i is the bulk free energy for the α and β phases, and the λ and C_i constants are the parameterization

variables chosen to match the work by Homer et al. (Table 1).

The general microstructural evolution for multi-state systems has been simulated by the PMC model [9], which we incorporate to calculate the sharp interfacial energy, given by

$$\int_{\mathcal{S}} \gamma_{Potts} dS \equiv J \sum_{i=1}^{N} \sum_{j=1}^{n} (1 - \delta_{s_i s_j}) \quad (6)$$

where J is the interaction energy between adjacent elements, n is the number of neighboring particles, δ is the Kronecker delta, and s_i and s_j are the grain id for the i and j sites. Then, introducing Eqs. (5) and (6) into Eqs. (1) and (3), we get the following discretized equations of state:

$$F_{hPPF} = \sum_{i=1}^{N} \left(f_0(q_i, C_i) + \frac{\gamma_{CH}}{2} |\nabla C_i|^2 + J \sum_{j=1}^{n} (1 - \delta_{s_i s_j}) \right) \quad (7)$$

$$F_{Potts} = \sum_{i=1}^{N} \left(f_0(q_i, C_i) + J \sum_{j=1}^{n} (1 - \delta_{s_i s_j}) \right). \quad (8)$$

To simulate grain growth and phase coarsening, we minimize the EoS by means of the standard Metropolis algorithm. For each site i, we choose a neighboring site j at random and attempt to adopt the neighbor's id and phase. The change is adopted following Boltzmann statistics. The probability of accepting the microstructural change is given by

$$P = \begin{cases} 1, & \Delta F \leqslant 0 \\ \exp\left(-\frac{\Delta F}{k_B T}\right), & \Delta F > 0 \end{cases} \quad (9)$$

where ΔF is the change of energy for the event calculated using Eq. (7) or (8), k_B is the Boltzmann constant and T is the absolute simulation temperature. For the concentration evolution, we use the phenomenological equation

$$\frac{\partial C}{\partial t} = \nabla \cdot (M \nabla \mu) \quad (10)$$

where μ is the chemical potential and M is the mobility. The chemical potential is defined as $\mu \equiv \delta F / \delta C$. Incorporating Eqs. (1) and (3) into Eq. (10) and non-dimensionalizing, for the hPPF model we get

$$\frac{\partial C}{\partial \tilde{t}} = \tilde{\nabla} \cdot \left[\tilde{\nabla} \left(\frac{\partial \tilde{f}_0}{\partial C} - \tilde{\nabla}^2 C \right) \right] \quad (11)$$

where $\tilde{t}, \tilde{\nabla}$ and $\tilde{f}_0$ are the non-dimensionalized time, spatial gradient and bulk chemical free energy, respectively. For our sharp interface model we get

$$\frac{\partial C}{\partial \tilde{t}} = \tilde{\nabla} \cdot \left[\tilde{\nabla} \left(\frac{\partial \tilde{f}_0}{\partial C} + \tilde{\kappa} \right) \right] \quad (12)$$