Allen–Cahn equation for multi-component crystal growth

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Abstract. We propose a multi-component Allen–Cahn equation for crystal growth. There are quite a few models for crystal growth in the literature. In particular, there are phase-field models inspired by the Allen–Cahn equation for a single crystal. We would like to extend such phase-field models for single crystals to multiple crystals. Under the k-fold symmetry, growth of multiple crystals is well modeled and simulated by our method. In particular, the merging phenomenon of nearby crystals is captured in our simulations.

Introduction

The Allen–Cahn equation introduced by Allen and Cahn [1],

$$u_t = \epsilon \Delta u + \frac{1}{\epsilon} W'(u),$$

is a well-known phase separation model with a double well potential $W(u) := \frac{(1-u^2)^2}{4}$. This is also interpreted as a gradient flow of the Ginzburg-Landau energy functional $E(u) := \frac{\epsilon}{2}\int_\Omega |\nabla u(\mathbf{x})|^2 d\mathbf{x} + \frac{1}{\epsilon}\int_\Omega W(u(\mathbf{x}))d\mathbf{x}$. When modeling multiple components, we use a phase variable $\phi = \phi_A + \phi_B$. Under the k-fold symmetry, we use the k-fold symmetric interfacial energy $\epsilon(\phi) = \epsilon_0(1 + \epsilon_k \cos(k\phi))$.

Results and Discussion

The model we propose is

$$\begin{aligned} \epsilon^2(\phi)\frac{\partial \phi}{\partial t} &= \nabla \cdot \left(\epsilon^2(\phi)\nabla\phi\right) - \left[\frac{2\phi - 1}{2} + \lambda u \frac{\phi(\phi-1)}{4}\right]\phi(\phi-1) + \text{div}(F(\phi)) + \beta(\phi), \\ \frac{\partial u}{\partial t} &= D\Delta u + \frac{1}{2}\frac{\partial \phi}{\partial t}, \end{aligned}$$

where $F(\phi) = \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_x}, |\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_y}\right)$ and $\beta(\phi)$ is defined by

$$\begin{aligned} \beta(\phi) := -\frac{1}{2}\Big[& 2\epsilon(\phi_A)\nabla\epsilon(\phi_A)\cdot\nabla\phi_A - W'(\phi_A) - 4\lambda u W(\phi_A) + \text{div}(F(\phi_A)) \\ &+ 2\epsilon(\phi_B)\nabla\epsilon(\phi_B)\cdot\nabla\phi_B - W'(\phi_B) - 4\lambda u W(\phi_B) + \text{div}(F(\phi_B))\Big]. \end{aligned}$$

Below are two simulation results. Unlike other models, our phase-field model can simulate the merging phenomenon of nearby crystals.

(a) Left: ϕ_A, Middle: ϕ_B, Right: $\phi = \phi_A + \phi_B$

(b) Crowded crystals with three phases

Figure 1: (a) 6-fold case, (b) 8-fold case

We will also present more numerical simulations and discuss comparison results.

References

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