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Coarsening Kinetics of a Two Phase Mixture with Highly Disparate Diffusion Mobility

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Abstract. The coarsening kinetics of a two-phase mixture with a large diffusional mobility disparity between the two phases is studied using a variable-mobility Cahn-Hilliard equation. The semi-implicit spectral numerical technique was employed, and a number of interpolation functions are considered for describing the change in diffusion mobility across the interface boundary from one phase to another. The coarsening rate of domain size was measured using both structure and pair correlation functions as well as the direct computation of particle sizes in real space for the case that the coarsening phase consists of dispersed particles. We discovered that the average size ($\overline{R}$) versus time (t) follows the $\overline{R}^{10/3} \propto t$ law, in contrast to the conventional LSW theory, $\overline{R}^3 \propto t$, and the interface-diffusion dominated two-phase coarsening, $\overline{R}^4 \propto t$.

AMS subject classifications: 65M70, 35F20, 81T80

Key words: Coarsening kinetics, Cahn-Hilliard equation, phase-field method, computer simulation.

1 Introduction

Coarsening is a kinetic process driven by the reduction in the total interfacial energy of a microstructure. As the mechanical properties of a material are critically determined

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by the degree of microstructure coarsening, it has been a subject of interest in materials science and engineering for over the last half century [1–4].

The first formal theory of coarsening was developed more than 40 years ago by Lifshitz and Slyozov [5], and Wagner [6], i.e. the so-called LSW theory which predicts that the cube of average particle size, $\overline{R}$, is linearly proportional to time t, i.e.,

$$\overline{R}^3-\overline{R}_0^3=kt,$$

where k is the rate constant and $\overline{R}_0$ is the average length at time t = 0, and the particle sizes normalized by the average size have a unique distribution which is independent of time. LSW theory assumes that precipitates are spherical and the volume fraction of the coarsening phase is zero. Many attempts to improve the LSW theory by relaxing the zero volume fraction assumption [Ardell [7], Tsumuraya and Miyata [8], Asimow [9], Sarian and Weart [10], Aubauer [11,12], Brailsford and Wynblatt [13], Voorhees and Glicksman [14], Marqusee and Ross [15], Tokuyama and Kawasaki [16], Marsh and Glicksman [17], and Davies et al. [18]] do not fundamentally change the cubic coarsening kinetics. The LSW cubic law for bulk-diffusion-dominated coarsening was confirmed by numerical simulations using a constant-mobility Cahn-Hilliard equation [19–22] which takes into the effect of non-spherical particle morphologies as well as volume fractions.

There have also been a number of studies using the Cahn-Hilliard equation with the scaled variable mobility term

$$M=1-aC^2,$$

where $C=C(\mathbf{r},t)$ is the compositional field, [Langer et al. [23], Kitahara et al. [24], Lacasta et al. [25] and Zhu et al. [26]] which allow one to model two common diffusion mechanisms: a constant mobility describing bulk-diffusion-dominated coarsening ($\overline{R}\propto t^{1/3}$) for $a=0$ and the coarsening dominated by interfacial diffusion for $a=1$. These works convincingly showed that the coarsening of a two-phase microstructure with predominantly interfacial diffusion leads to $\overline{R}^4\propto t$ [27] power law while for all other values of a between 0 and 1 ($a\neq 1$), there is a cross-over between $\overline{R}\propto t^{1/3}$ and $\overline{R}\propto t^{1/4}$. Based on dimensionality argument, Bray et al. [28] derived a growth law

$$\overline{R}^{(3+\alpha)}\propto t$$

corresponding to the Cahn-Hilliard equation with a composition-dependent-mobility,

$$M\propto(1-C^2)^{\alpha},$$

in the Lifshitz-Slyozov limit where the minority phase occupies a vanishingly small volume fraction. This theory successfully predicted two classic coarsening kinetics regimes: $\alpha=0$ for diffusion-limited coarsening and $\alpha=1$ for interfacial diffusion dominated coarsening.