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Effect of volume fractions on microstructure evolution in isotropic volume-conserved two-phase alloys: A phase-field study

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ABSTRACT

A detailed investigation was carried out to study the effect of volume fraction on microstructure evolution in segregation-free isotropic volume-conserved two-phase alloys. Large scale two-dimensional (2D) and three-dimensional (3D) simulations were performed for 10/90, 30/70 and 50/50 alloys with a modified quantitative phase-field model. The grain growth in the two-phase alloys was consistent with volume-diffusion controlled growth with growth exponent $m \sim 3$. The kinetic coefficient, mean grain size, mean number of faces, grain size distribution (GSD), grain topology distribution (GTD) and grain size/topological class relation were all influenced by the volume fraction of the minor phase (α) in the two-phase alloys. In the 10/90 alloy, a bimodal distribution in the GSD and GTD for the 2D total grain structure was found. The timelines of evolution of major-phase grains in 3D simulations for all alloys were examined. 'Particle-like' grain migration of isolated α-phase grains was observed in the 2D simulations. The formation and evolution of non-constant curvatures on interphase boundaries in the isotropic volume-conserved two-phase alloys is discussed. The microstructure evolution in the volume-conserved two-phase alloys was compared with that in non-conserved two-phase alloys ($m \sim 2$). Simulation results are found to be in good agreement with a wide range of previous experimental and computer simulation results.

1. Introduction

Microstructure evolution in single-phase systems has been extensively investigated through analytical, experimental and computational studies [1–5]. However materials with a two-phase microstructure often offer better material properties like high strength, toughness and corrosion resistance, over single-phase materials. Two-phase microstructures are therefore desired in many important materials like Al_2O_3–ZrO_2 ceramic composites, titanium alloys and duplex stainless steel. The growth kinetics in two-phase alloys is expected to follow a power law,

$$\langle R_t \rangle^m - \langle R_0 \rangle^m = K * t \tag{1}$$

where $\langle R_0 \rangle$ is initial mean grain size, m is grain growth exponent, K is kinetic coefficient and t is time. The growth exponent (m) varies depending on the dominant growth mechanism, namely interface controlled growth ($m = 2$), volume-diffusion controlled growth

($m = 3$) and grain-boundary diffusion controlled growth ($m = 4$) [4,5].

A two-phase microstructure consisting of α and β phases may contain α/α and β/β grain boundaries between two α and two β phase grains respectively along with α/β interphase interfaces between α and β grains. The evolution of both phases is mutually constrained in a two-phase microstructure due to space filling requirements. According to Cahn [6], the energetic ratios E_α and E_β, where E is the ratio of the grain boundary energy (σ_α or σ_β) to the interphase boundary energy ($\sigma_{\alpha\beta}$), determine microstructure evolution and characteristics in two-dimensional two-phase microstructures. This was later confirmed by Holm et al. [7], who carried out 2D simulations using a Monte Carlo-Potts model for non-conserved two-phase systems for various E-values. Ohnuma et al. [8] studied 2D simulations for volume-conserved two-phase systems using a modified Monte Carlo-Potts model and observed a growth exponent $m \sim 3$. Solomatov et al. [9] carried out 2D Monte Carlo simulations in the grain boundary diffusion controlled growth regime ($m \sim 4$) for volume-conserved two-phase systems. Fan and Chen [10–12] performed 2D phase-field simulations for volume-conserved two-phase systems and found that volume-diffusion ($m \sim 3$) is the dominant growth mechanism. [11] also

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observed that the kinetic coefficient (K) depends on the energetic ratios E_α and E_β, initial microstructure and the volume fractions of the phases for volume-conserved two-phase alloys. Homer et al. [13] proposed a hybrid Potts-phase field model for volume-conserved two-phase systems. Poulsen et al. [14] carried out 3D simulations of the evolution of volume-conserved two-phase alloys using a modified Fan-Chen phase-field model for $E_\alpha = E_\beta = 0.8$ where interphase boundaries (α/β) are less favorable than the α/α and β/β grain boundaries. Various experimental investigations of microstructure evolution in two-phase metallic systems and ceramic composites found that the growth exponent m is in the range of 2–4 [15–19].

Previous experimental studies [15–20] and Monte Carlo simulations [8,9,13] however provide very limited or no information on the effect of volume fractions on the mean number of faces, the grain size distribution (GSD), the grain topology distribution (GTD) and the grain size/topology class relationship in 2D or 3D two-phase systems. Moreover, solute segregation at the grain boundaries and triple junctions is unavoidable in the phase-field models proposed by Chen and Fan [10], Poulsen et al. [14]. Poulsen et al. [14] studied the effect of solute segregation on grain boundaries and concluded that the motion of grain boundaries was not affected by the presence of solute segregation in their simulations. However they did not report on the effects of solute segregation on the motion of triple junctions. The effect of solute segregation at grain boundaries and triple junctions on the GTD and grain size/topology class relationship is in general not clearly understood. In some of the previous 2D phase-field simulations of two-phase coarsening [10–12], coalescence of same-phase grains was unavoidable [21]. Finally, the simulations carried out by Poulsen et al. [14] are limited to only two alloys (40/60 and 50/50) which may not be sufficient to understand the effect of volume fraction on microstructure evolution in the volume-conserved two-phase alloys.

The purpose of this paper is to study the effect of the volume fraction of the minor phase on microstructure evolution in segregation free isotropic volume-conserved two-phase systems in 2D and 3D. A modified quantitative phase-field model is employed to investigate the growth kinetics and topological evolution in 10/90, 30/70 and 50/50 (vol%) two-phase alloys. All simulations are carried out for systems with $E_\alpha = E_\beta = 1$. A 'time-line' study of the evolution of the major-phase grains in all alloys is performed. The observed 'particle-like' grain migration of the minor phase grains and bimodal distribution in the 10/90 alloy are also discussed. Furthermore, the presence of a non-constant curvature along the isotropic interphase boundaries and how it evolves towards a constant curvature in the volume-conserved two phase systems was analyzed. The microstructure evolution in volume-conserved two-phase systems is also compared with that in an isotropic non-conserved two-phase system with equal volume fractions. The findings from the simulations are compared with previously published simulations and experimental results.

2. Phase-field model

2.1. Phase-field variables

A binary two-phase system A-B consisting of α and β grains is assumed. The molar fraction of component B, as a function of time and space, is represented by $C(\mathbf{r},t)$. As in the two-phase models of Chen and Fan [10] and Poulsen et al. [14], the different grain orientation in the α and β phases are represented by $\eta_{1\ldots r}(\mathbf{r},t)$ and $\eta_{r+1\ldots p}(\mathbf{r},t)$ respectively. Within each grain one of the η_i equals 1, while all $\eta_{i\neq 1}$ equal 0. At the interface between

2 grains, the $\eta_{1\ldots p}$ change their value smoothly within a small, but finite, interface region. It is assumed that the molar volume V_m is the same in both phases and does not depend on composition. Simulations are performed at constant temperature and pressure.

2.2. Free energy formulation

The total free energy functional used in this study is given by

$$F = \int_V \left[f_{interf}(\eta_i) + f_{chem}(\eta_i, C) \right] dV \tag{2}$$

where f_{interf} is only different from 0 near the interfaces and f_{chem} only contributes to the chemical bulk energy and not to the interfacial energy. The interfacial energy part is based on [22] with the modifications and parameter relations from [23]

$$f_{interf} = m \left[\sum_{i=1}^{p} \left[\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right] + \gamma \sum_{i=1}^{p} \sum_{j=i+1}^{p} \eta_i^2 \eta_j^2 + \frac{1}{4} \right] + \frac{\kappa}{2} \sum_{i=1}^{p} (\nabla \eta_i)^2 \tag{3}$$

where κ, m and γ are coefficients related to the interface energy and width of the interface region. It was derived that, for $\gamma = 1.5$, the relation between interface energy and the coefficients κ and m is $\sigma = \left(\sqrt{2}/3 \right) \cdot \sqrt{m \cdot \kappa}$ [23].

For the chemical energy f_{chem}, the formulation of [24] is adopted

$$f_{chem} = \frac{A}{2} \left(C - \phi_\alpha C_{o,\alpha} - \phi_\beta C_{o,\beta} \right)^2 \tag{4}$$

where $C_{o,\alpha}$ and $C_{o,\beta}$ are the equilibrium compositions of the α and β phase at the considered temperature. The parameter A determines the steepness of the parabolic free energy. The ϕ_α and ϕ_β are the local phase fractions, which can be calculated from the $\eta_{1\ldots r}$ and $\eta_{r+1\ldots p}$ as $\phi_\alpha = \sum_{i=1}^{r} \eta_i^2 / \sum_{i=1}^{p} \eta_i^2$ and $\phi_\beta = \sum_{i=r+1}^{p} \eta_i^2 / \sum_{i=1}^{p} \eta_i^2$ [25].

This formulation is limited to parabolic free energies which is an acceptable simplification for coarsening simulations, since the phase compositions will not deviate much from the equilibrium phase compositions in bulk materials. Formulation (4) from [24] ensures that the chemical part f_{chem} in (2) does not affect the interfacial energy in the phase-field model and avoids solute segregation at the grain boundaries. Hence the motion of $\alpha\alpha\alpha$ and $\beta\beta\beta$ triple junctions in grain clusters of a same-phase is not affected by the diffusion fluxes of segregated solute, as may have been the case in previous phase-field models [10,14].

2.3. Governing equations

Composition is a conserved quantity and its evolution can be modeled with the following differential equation [25]

$$\frac{\partial C}{\partial t} = -\nabla \cdot \left[-M(\eta_i) \nabla \frac{\partial f_{chem}}{\partial C} \right] \tag{5}$$

where $M(\eta_i)$ is the diffusion mobility calculated as $M(\eta_i) = \phi_\alpha M_\alpha + \phi_\beta M_\beta$. The diffusion mobilities of the two phases (M_α and M_β) are calculated as $M_\alpha = D_\alpha/A$ and $M_\beta = D_\beta/A$ where the D_α and D_β are the interdiffusion coefficients of α and β phases respectively and f_{chem} as given in Eq. (4).

Evolution of the non-conserved phase field variables η is given as [25]

$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta F}{\delta \eta_i} \tag{6}$$

where L is a kinetic coefficient. The parameters L, κ, m and γ can be related to material properties of the two-phase systems in order to perform quantitative simulations [23,25]. In this study, L is chosen the same for all boundaries and so that the movement of the