Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 56 (2008) 4585–4592
Acta MATERIALIA
www.elsevier.com/locate/actamat

Phase-field modeling of isothermal dendritic coarsening in ternary alloys

Jincheng Wang *, Gencang Yang

State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Youyi West Road 127#, Xi'an, Shaanxi Province 710072, PR China

Received 31 March 2008; received in revised form 30 April 2008; accepted 13 May 2008
Available online 24 June 2008

Abstract

The process of isothermal dendritic coarsening in a Ni–Al–Nb ternary system is simulated by using the phase-field method. The coarsening behaviors and coarsening mechanisms with different solid fractions f_S are investigated in detail. Simulated results show that, as f_S increases from 64% to 88%, the coarsened morphology of the liquid phase varies from connected plate to rod-like shape, which is similar to the lamellar to rod transition in eutectics due to the interface energy. Simulated results also indicate that the dendritic isothermal coarsening mechanisms are dominated by remelting of the third arms, coalescence and smoothing in the case of low solid fraction, while in the case of high solid fraction, coalescence, smoothing, Rayleigh instability, rounding and shrinking away of small liquid droplets are the main mechanisms of dendritic coarsening. The increase of liquid diffusion coefficient D^L will also trigger the Rayleigh instability to accelerate the morphology transition from plate to cylindrical for the liquid phase.

Keywords: Phase-field method; Dendritic coarsening; Ternary alloys; Coarsening mechanism

1. Introduction

Coarsening occurs in a vast array of two-phase systems and is driven by the interfacial curvature, resulting in a decrease in the interfacial area per unit volume and an concomitant increase in the scale of the interfacial morphology [1–7]. The coarsening behavior affects the distribution of length scales, microsegregation and other microstructural characteristics of the materials, all of which determine the physical and chemical properties of the materials in terms of strength, ductility, electrical conductivity and corrosion resistance. Therefore, a complete understanding of the phase-coarsening process would improve the design of process parameters and the overall control of the final microstructures.

In ramified dendritic microstructures, the coarsening process is as evident as in uniformly dispersed systems of near-spherical particles [3–7]. The dendrites undergo a coarsening process that determines their ultimate morphology and length scale, which in turn are crucial to the mechanical properties of the final ingot. However, research on dendritic coarsening has been, until recently, restricted to the examination of either individual dendrites in transparent systems or planar sections through the dendritic structure in opaque systems. Marsh [3] pointed out that dendritic coarsening can be described as a relaxation process driven by the thermodynamics of the interfacial surface energy in a two-phase structure. Kattimis et al. [5] and Young and Kirkwood [6,7] have investigated the coarsening behavior of dendritic structures in Al–Cu alloys. Huang and Glicksman [8,9] did experiments with succinonitrile dendrites and concluded that isothermal coarsening during dendritic solidification occurs by competitive side branch growth. Li et al. [10] used an improved synchrotron microradiography technique to study dendrite growth and coarsening in Sn–13%Bi alloy in real time. Coarsening mechanisms such as dendrite arm remelting from tips to roots, coalescence by local solidification at liquid grooves between side arms, and fragmentation have also been observed. Recently, Voorhees's research group has made significant progress in studying the dendritic

* Corresponding author. Tel.: +86 29 88460650; fax: +86 29 88492374.
E-mail address: jchwang@nwpu.edu.cn (J. Wang).

1359-6454/$34.00 © 2008 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.actamat.2008.05.016

coarsening process [11–17]. These researchers have shown that topological measurements can be used to quantitatively describe the evolution of the interfacial morphology during coarsening using three-dimensional reconstructions.

As for the dendritic coarsening mechanisms, as shown in Fig. 1 [11], a number of coarsening models, i.e. radial melting (model I), fragmentation (model II), axial melting (model III) and coalescence (models IV and V) have been proposed to explain certain phenomenological aspects of the coarsening process. These models involve mass transport driven by the Gibbs–Thomson effect, i.e. the difference in local curvature of the liquid–solid interface results in the surfaces with high curvature melting due to the depression in the liquidus temperature and those surfaces with low curvature tending to grow coarser by diffusion. In general, these models employ an oversimplified dendritic morphology and are limited to the consideration of the localized evolution of dendrites. To formulate more realistic models, information on the complete topology of the dendritic structure and its evolution is required. Moreover, all these dendritic coarsening models are based on the fact that liquid phase is the matrix phase, which means that the solid fraction in the liquid–solid system is relatively low. When the solid fraction is very high and the solid phase acts as the matrix phase, the coarsening mechanism is obviously different.

On the one hand, the fact that two-phase mixtures can have both complex morphologies and behavior is a long way from that predicted by the classical mathematical models developed for dispersions of spherical particles. Being an elegant and integrated simulation technique, the phase-field method has been successfully employed as a powerful tool for describing and predicting the morphological evolution of complex solidification structures [18,19]. Phase-field calculation provides a useful tool for describing the dendritic coarsening process and elucidating the coarsening mechanisms and behaviors [20,21]. Using the phase-field method, Warren and Boettinger [22,23] obtained realistic growth patterns including the development, coarsening and coalescence of secondary and tertiary dendrite arms. Mendoza et al. [11] also coupled theory and experiment by using the experimentally measured three-dimensional microstructure as an initial condition for phase-field calculations. The above research efforts demonstrate that the phase-field method is a powerful tool not only in dendritic growth but also in dendritic coarsening. In addition, Wu [20] has pointed out that phase-field simulation may be the best tool for predicting the coarsening behavior of morphologically complex systems. However, very few studies, especially systematic work on the isothermal dendritic coarsening behaviors and mechanisms, have been done.

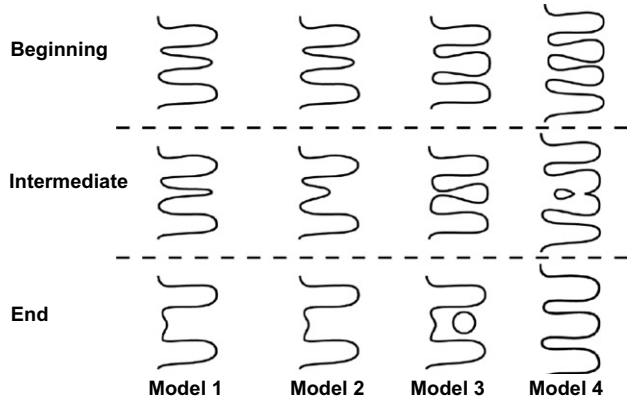

Fig. 1. Four models for isothermal coarsening: (1) radial remelting, (2) axial remelting, (3) arm separation, and (4) coalescence of two dendrite arms [11].

On the other hand, multicomponent alloy systems are an important class of materials, especially for technical applications and processes. The solidification of multicomponent alloys is a central part of many industrial processes and natural phenomena. Recently, phase-field models have been extended to multicomponent alloy systems via coupling of the phase-field equations to thermodynamic databases and equilibrium calculations [23–26]. Therefore, in the present paper, the phase-field method is employed to study the dendritic coarsening behaviors and mechanisms in a ternary system with an emphasis on the effects of the solid fraction on the coarsening process and coarsening mechanisms.

2. Phase-field model

2.1. Governing equations

In the present paper, the multicomponent phase-field model proposed by Kobayashi et al. [25] is adopted. For a ternary A–B–C system, if the liquid phase and the solid phase (usually a solid-solution phase) can be described by an extended regular solution approximation to define the free energy density, the Gibbs energy for the liquid phase and the solid phase can be expressed as

$$G_{\varphi}^{\mathrm{reg}}(c_1^{\varphi},c_2^{\varphi},c_3^{\varphi}) = \sum_{j=1}^{3}(c_j^{\varphi}G_j^{\varphi}) + RT\sum_{j=1}^{3}c_j^{\varphi}\ln c_j^{\varphi} + \sum_{j=1}^{3}\sum_{i>j}^{3}c_i^{\varphi}c_j^{\varphi}L_{i,j}^{\varphi} + c_1c_2c_3L_{1,2,3}^{\varphi}, \quad \varphi = \mathrm{L},\mathrm{S}, \tag{1}$$

where the subscript φ stands for liquid phase (L) or solid phase (S) and the subscripts 1, 2, 3 represent the elements A, B and C, respectively. G^{φ} and L^{φ} are thermodynamic parameters.

The free energy density consists of the free energy of the bulk phases and an imposed parabolic potential $g(\varphi)$ which is given by $\varphi(1-\varphi)$ and can be written as

$$f(\phi,c_1,c_2) = h(\phi)f^{\mathrm{S}}(c_1^{\mathrm{S}},c_2^{\mathrm{S}}) + [1-h(\phi)]f^{\mathrm{L}}(c_1^{\mathrm{L}},c_2^{\mathrm{L}}) + wg(\phi), \tag{2}$$