Phase-field simulation of abnormal grain growth due to inverse pinning

Yoshihiro Suwa [a,*], Yoshiyuki Saito [b], Hidehiro Onodera [c]

[a] *Computational Materials Science Center, National Institute for Materials Science, Tsukuba 305-0047, Japan*
[b] *Department of Materials Science and Engineering, Waseda University, Tokyo 169-8555, Japan*
[c] *Materials Engineering Laboratory, National Institute for Materials Science, Tsukuba 305-0047, Japan*

Abstract

The possibility of abnormal grain growth due to inverse pinning was verified using phase-field simulations. In bicrystalline systems with circular precipitates, the perfect wetting condition is required for the long-distance migration of the interface between the matrix grains. If the distance between precipitates that are perpendicular to the interface exceeds a critical value, the migration is not observed irrespective of the wetting condition. In polycrystalline systems, abnormal grain growth occurs with the aid of the driving force for grain growth even though l_{lim} exceeded the critical value, where l_{lim} is the minimum distance between precipitates. Furthermore, the perfect wetting condition is not required for the abnormal grain growth in the polycrystalline systems. These facts enlarge the possibility of inverse pinning in real alloy systems.

© 2007 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Computer simulation; Abnormal grain growth; Pinning; Phase-field modeling

1. Introduction

The grain growth processes that occur in polycrystalline materials during annealing are usually classified into two types. The first type is a self-similar coarsening process, which is called normal grain growth. In normal grain growth, an invariant distribution of scaled grain sizes develops, and the grain growth obeys a power-law kinetics with a characteristic exponent of 1/2 [1–20]. The second type is called abnormal grain growth and is characterized by the coarsening of a few grains at the expense of the surrounding matrix. In such conditions, the self-similar aspect of the coarsening process is lost.

Different mechanisms have been proposed for abnormal grain growth, although the actual physical mechanism responsible for this phenomenon remains largely unknown. Defect-induced strains can induce isolated grain growth [21], as well as the same capillary forces responsible for coarsening when anisotropy of grain boundary energies

or mobilities exists [22,23]. The conditions for abnormal growth due to variable interfacial energies or mobilities were recently examined [24,25] using a mean-field treatment of the matrix grains. For the case of a single grain with boundary properties that differ from those of the surrounding matrix, it was found that higher boundary mobility generally promotes abnormal growth whereas higher boundary energy constrains it. The detailed behavior can be quite complex, depending on the ranges of the model parameters selected. This includes abnormal growth only up to a limiting grain size, or lower bounds in the initial relative size of the grain for abnormal growth to occur. Abnormal grain growth has also been shown to occur when grain boundaries pin due to, for example, existing precipitate phases or other defects. Simplified models have been proposed that introduce grain boundary drag forces that lead to ultimate pinning (Zener pinning) [26–28], while the role of thermal fluctuations in overcoming pinning has been analyzed by Monte Carlo simulation [29].

Dispersed precipitates have been generally considered to be the inhibitors for boundary migration. However, it is assumed that, when anisotropic precipitates are present in

* Corresponding author.
E-mail address: suwa.yoshihiro@nims.go.jp (Y. Suwa).

the matrix and the boundary energy of these precipitates in a grain of type I is smaller than that in the adjacent grain of type II (for simplicity, we consider bicrystalline sample), the grain boundary between two grains is induced to migrate by these precipitates. Nishizawa called this phenomenon "inverse pinning" [30].

Nishizawa suggested that a typical example of inverse pinning was observed in steels when AlN precipitates were present. The AlN is an anisotropic ionic compound with a hexagonal B4 structure that precipitates in steel in the form of platelets or fine needles along specific planes of the parent metallic crystals. Consequently, the selective growth of a favorably oriented grain of type I occurs due to inverse pinning if it has the same orientation as the parent crystal of the group of AlN. In addition, Miodownik [31] suggests that it is very much an open question whether pinning force anisotropy (i.e. the boundary energy is a strongly anisotropic function of boundary plane and/or misorientation) is the cause of abnormal growth or preferred orientations in some systems, leading to strong textures and the attendant misorientation distribution function of nanocrystalline nickel alloys and Fe–Si systems [32].

The main purpose of this study is to verify the possibility of abnormal grain growth due to inverse pinning by using phase-field simulations. All calculations will be performed on a two-dimensional (2D) lattice with a periodic boundary condition. For simplicity, it is assumed that there exist only two groups of orientations (A) and (B) for matrix grains and one for precipitates (P). The system with a single texture component (A) in a matrix of randomly oriented grains (B) is considered. Further, we assume that the precipitates (P) have a special orientation relationship with A, where the difference in the boundary properties of A/A, A/B, and B/B boundaries is not introduced to emphasize the effects of inverse pinning. We evaluate whether a preferred growth of A grains occurs or not, provided that only interfaces BP have a higher boundary energy and the other interfaces have equivalent and smaller boundary energies. We will perform numerical simulation for bicrystalline systems in Sections 3.1–3.3 and for polycrystalline systems in Sections 3.4 and 3.5.

A numbers of simulations with finely dispersed precipitates have been performed using Monte Carlo Potts models [29,33–41], the vertex model [42,43] and the phase-field model [41,44–46]. However, for both experiments and numerical simulations, there have been no systematic investigations of anisotropic pinning. In experiments, it is difficult to change the volume fraction of precipitates and their distribution without changing other variables, such as composition. In numerical simulation, in order to treat the anisotropy in precipitate–matrix interfaces precisely, a higher spatial resolution is required that requires huge computational costs.

Systematic investigations have been feasible, provided the volume fraction of precipitates is relatively high [47,48]. However, the computational costs for obtaining statistically meaningful results become higher with decreasing volume fraction. In this study, for realizing the simulation with the anisotropy in precipitate–matrix interfaces, we utilize an efficient algorithm called the active parameter tracking (APT) algorithm [49–51] coupled with parallel coding techniques. This enables us to perform large-scale calculations, such as 2048^2 grid points.

2. Method

2.1. Phase-field model

To represent the temporal evolution of polycrystalline material with finely dispersed precipitates we utilized the multi phase-field (MPF) model proposed by Steinbach and Pezzola [52]. In this paper, a set of continuous field variables, $\phi_1(\mathbf{r}, t)$, $\phi_2(\mathbf{r}, t)$, ..., $\phi_N(\mathbf{r}, t)$, are defined to distinguish the types of constituents (matrix grains and precipitates) and their orientation, where $\phi_i(\mathbf{r}, t)$ represents the existence ratio of each constituent at a position $\mathbf{r}$ and time t. As described in Section 2.2, in order to avoid the coalescence of constituents that have the same field number i, we apply a unique number to each constituent (i.e. N is assumed to be the total number of constituents). We derive governing equations according to Ref. [53] as follows:

The sum of phase fields at any position in the system is conserved.

$$\sum_{i=1}^{N} \phi_i(\mathbf{r}, t) = 1 \tag{1}$$

The free energy functional of a system of volume V is given by

$$F = \int_V \left[f^P + f^T + \lambda_L \left(\sum_i^N \phi_i - 1 \right) \right] dV \tag{2}$$

where λ_L is the Lagrange multiplier accounting for the constraint Eq. (1) and f^P can be defined by

$$f^P = \sum_{j>i}^{N} \sum_{i}^{N} \left[-\frac{\epsilon_{ij}^2}{2} \nabla \phi_i \cdot \nabla \phi_j + \omega_{ij} \phi_i \phi_j \right] \tag{3}$$

as in Steinbach and Pezzola [52], where ϵ_{ij} is the gradient energy coefficient and ω_{ij} is the height of the double-well potential. The parabolic double-well potential $\phi_i \phi_j$ is defined in the boundary region only where $0 < \phi_i < 1$ and $0 < \phi_j < 1$. For the thermodynamic potential f^T, we assume a rule of mixture

$$f^T = \sum_i^N \phi_i f^i(c_i) \tag{4}$$

where $f^i(c_i)$ is the free energy density of phase i with composition c_i. Any point (x, y) in the system is assumed to be a mixture of N phases, with the fraction of ϕ_i for phase i. However, the compositions of the phases coexisting at a given point are not independent of each other, but are constrained by the following condition [54]: