



Zener pinning through coherent precipitate: A phase-field study

Tamoghna Chakrabarti^{a,*}, Sukriti Manna^{b,*}

^a Department of Metallurgical & Materials Engineering, Indian Institute of Technology Patna, Patna 801106, India

^b Department of Mechanical Engineering, Colorado School of Mines, Golden, CO 80401, USA



ARTICLE INFO

Keywords:

Misfit
Coherent precipitate
Grain size
Phase-field
Zener pinning

ABSTRACT

A novel phase field model has been developed to study the effect of coherent precipitate on the Zener pinning of matrix grain boundaries. The model accounts for misfit strain between precipitate and matrix as well as the elastic inhomogeneity and anisotropy between them. The results show that increase in elastic misfit, elastic inhomogeneity, and elastic anisotropy increases the coarsening rate of the precipitates. Increased coarsening of precipitates in turn decreases the pinning of grain boundaries. Therefore, increase in misfit strain, elastic inhomogeneity and anisotropy mostly negatively affect the Zener pinning through coherent precipitate. This study shows elastic anisotropy gives rise to the needle shape precipitate. It has also been shown that these needle shaped precipitates are not very effective in Zener pinning. This study provides an understanding into the effect of coherent precipitate on the Zener pinning of matrix grain boundaries. To design a material with smallest possible grain size, coherent precipitate with least lattice misfit and highest elastic modulus will be most effective.

1. Introduction

The grain size and morphology in polycrystalline materials often play an important role in determining the properties of materials. A wide gamut of material properties such as yield strength [1] and ultimate tensile strength [2], creep [3], fracture resistance [4], oxidation [5], corrosion resistance [6,7], electrical [8], magnetic [9], and optical [10], properties can be altered by modifying the grain size and morphology. In systems such as aluminum [11,12], aluminum based alloys [13], micro-alloyed steels [14], and nickel based superalloys [15], reduction in grain size improves the mechanical strength. Thus, it is imperative to understand the external factors such as solute segregation, precipitate nucleation or second phase addition by which we can control grain sizes and morphology to obtain desired properties depending on applications.

One of the simplest and possibly the most profound way of controlling the grain size is by means of introducing second phase in form of particles or precipitates [16]. The role of second phase particles or precipitates on the refining of the grain size has been first proposed by Smith and Zener [17,18]. This effect which is called Zener pinning works by pinning the grain boundaries at the particle-grain interface. In Zener pinning, second phase size, morphology, volume fraction, coherency, anisotropic interfacial energy and even the coarsening rate of the second phase particle affect the final pinning [19].

Theoretical models have been extensively employed to understand the interactions of these afore mentioned parameters in Zener pinning. Different computational techniques such as Monte-Carlo Potts models [20], front-tracking-type models [21], and phase field models [22,23] has been used to understand the Zener pinning phenomenon. Among these simulation techniques, we concentrate on phase field model to understand the Zener pinning phenomenon. The phase field model is a diffuse-interface model where the evolution of arbitrary complex grain and precipitate morphologies can be studied without any presupposition on their shape or distribution. Additionally, phase field model simulation results have also shown to be qualitatively consistent with experimental observations in many different types of systems and problems [24–29].

Previously through phase field model, the effect of volume fraction, shape, size, anisotropy and coarsening of the second phase particles on Zener pinning has already been studied in detail [21,30,23]. One of the important aspect to consider is the coherency of the second phase particles in Zener pinning which has not been studied in much detail. Due to coherency between the precipitate and matrix, the misfit strain can induce elastic stress, which can alter the coarsening behavior of the precipitates. Changes in the coarsening kinetics of the precipitate in turn can influence the Zener pinning drag.

Wang *et al.* [31] have investigated through a phase field model the effect of misfit strain of the Zener pinning by coherent precipitates. In

* Corresponding authors.

E-mail addresses: tamoghna@iitp.ac.in (T. Chakrabarti), smanna@mines.edu (S. Manna).

that model, the inhomogeneity in modulus between the matrix and second phase particles was not included. But, in practical applications, the precipitate modulus can be significantly different from that of the matrix phase. Such inhomogeneity in elastic modulus can in turn change the coarsening kinetics which has been implemented in our model. Additionally, we have inspected the effect of anisotropy in the elastic modulus which has a significant influence in changing the precipitate morphology from globular to needle shape.

Our article is organized as follows: In the Section 2, we present the details our phase field model. In the Section 3, we have discussed the results of our phase field simulations by systematically investigating the effect of misfit strain, elastic inhomogeneity, and anisotropy on grain coarsening kinetics. Additionally, we have studied the effect of different particle morphology which arises from the elastic anisotropy. Finally, the Section 4 contains the succinct conclusions of our work.

2. Methods

In our phase field model, the microstructure consists of two phases *i.e.* matrix and second phase particles (or precipitates). There exists a misfit between second phase and matrix. The matrix is polycrystalline whereas precipitate is single crystalline.

2.1. Free energy functionals

The total free energy (F_t) of system described by the sum of chemical energy (F_{ch}) and elastic energy (F_{el}) *i.e.* $F_t = F_{ch} + F_{el}$. F_{chem} of the system with inhomogeneities in the field of $c(\mathbf{r}, t)$ and $\eta_i(\mathbf{r}, t); i = 1, 2, \dots, n$ describes n unique grain orientations in the matrix phase is given by,

$$F_{ch} = N_v \int_v [f_0(c, \eta_i) + \kappa_c (\nabla c)^2 + \sum_{i=1}^n \kappa_i^\eta (\nabla \eta_i)^2] dv \quad (1)$$

where N_v : number of molecules per unit volume, $f_0(c, \eta_i)$: bulk free energy density, κ_c : gradient energy co-efficient due to composition $c(\mathbf{r}, t)$ variable, κ_i^η : gradient energy coefficient due to order parameter $\eta_i(\mathbf{r}, t)$ variable, v : volume of our domain of interest, \mathbf{r} : real space vector. The bulk free energy density $f_0(c, \eta_i)$ is given by [25],

$$f_0(c, \eta_i) = Ac^2(1-c)^2 + Bc^2\zeta(\eta_i) + Z(1-c)^2 \sum_{i=1}^n \eta_i^2 \quad (2)$$

where $\zeta(\eta_i)$ is expressed as [25],

$$\zeta(\eta_i) = \sum_{i=1}^n \left[\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} + 2 \sum_{j>i}^n \eta_i^2 \eta_j^2 \right] + 0.25 \quad (3)$$

and the parameters A, B, Z in Eq. (2) are constants.

2.2. Elastic energy

In our phase field model, the source of misfit arises due to the compositional heterogeneity between the matrix and precipitate. This misfit introduces the elastic energy in the system. The elastic energy contribution of the total free energy is given by,

$$F_{el} = \frac{1}{2} \int_v \sigma_{ij}^{el}(\mathbf{r}) \epsilon_{ij}^{el}(\mathbf{r}) dv \quad (4)$$

where $\sigma_{ij}^{el}(\mathbf{r})$: elastic stress tensor, $\epsilon_{ij}^{el}(\mathbf{r})$: elastic strain tensor and $\epsilon_{ij}^{el}(\mathbf{r})$ given by following equation,

$$\epsilon_{ij}^{el} = \epsilon_{ij}(\mathbf{r}) - \epsilon_{ij}^0(\mathbf{r}) \quad (5)$$

where $\epsilon_{ij}^0(\mathbf{r})$: position dependent eigenstrain, $\epsilon_{ij}(\mathbf{r})$: total strain which is given by following equation,

$$\epsilon_{ij}(\mathbf{r}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right) \quad (6)$$

Assuming that, there is no rotational component to the displacement field and phases obey the Hooke's law (*i.e.* both phases are linear elastic). Hence,

$$\sigma_{ij}^{el}(\mathbf{r}) = C_{ijkl}(\mathbf{r}) \epsilon_{kl}^{el}(\mathbf{r}) \quad (7)$$

where $C_{ijkl}(\mathbf{r})$: elastic modulus tensor. Now substituting the values of $\epsilon_{ij}^{el}(\mathbf{r})$ from Eq. (7) we obtain,

$$\sigma_{ij}^{el}(\mathbf{r}) = C_{ijkl}(\mathbf{r}) \{ \epsilon_{kl}(\mathbf{r}) - \epsilon_{kl}^0(\mathbf{r}) \} \quad (8)$$

As the stress field obeys the equation of mechanical equilibrium. Hence,

$$\begin{aligned} \sigma_{ij,j}^{el}(\mathbf{r}) &= 0 \\ \text{i.e. } \frac{\partial}{\partial r_j} [C_{ijkl}(\mathbf{r}) \{ \epsilon_{kl}(\mathbf{r}) - \epsilon_{kl}^0(\mathbf{r}) \}] &= 0 \end{aligned} \quad (9)$$

eigen strain, $\epsilon_{ij}^0(\mathbf{r})$ expressed as,

$$\epsilon_{ij}^0(\mathbf{r}) = \theta^c(c) \epsilon^c \delta_{ij} \quad (10)$$

here $\theta^c(c)$ is a shape function which is approximated as a linear function (following Vegard's law[32]) and expressed as,

$$\theta^c(c) = \frac{c(\mathbf{r}) - c^{ppt}}{c^{ppt} - c^{mat}} \quad (11)$$

$\theta^c(c)$ give value 1.0 at precipitate and 0.0 at matrix. In between particle and matrix (interface region), it takes values in between 1.0 and 0.0, ϵ^c : misfit strain between precipitate and matrix, δ_{ij} : Kronecker delta.

We are solving the equations for a plane strain approximation *i.e.* there is no eigenstrain in the z -direction.

2.3. Kinetics of microstructure evolution

We numerically solve Cahn–Hilliard equation for the evolution of composition $c(\mathbf{r}, t)$ and Allen–Cahn equation for order parameters $\eta_i(\mathbf{r}, t)$.

Cahn–Hilliard equation[33] is given by,

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \mu \quad (12)$$

M is mobility and is not a function of composition (c) and order parameter (η), μ is chemical potential and defined as,

$$\mu = \frac{\delta}{\delta c} (F/N_v) = \frac{\delta}{\delta c} (F_{ch}/N_v) + \frac{\delta}{\delta c} (F_{el}/N_v) \quad (13)$$

Here, $\frac{\delta}{\delta c}$ represents the variational derivative with respective to composition.

$$\frac{\delta}{\delta c} (F_{ch}/N_v) = \frac{\partial f_0}{\partial c} - 2\kappa_c \nabla^2 c \quad (14)$$

The final form of Cahn–Hilliard equation will be,

$$\frac{\partial c(\mathbf{r}, t)}{\partial t} = M \nabla^2 \left(\frac{\partial f_0}{\partial c} - 2\kappa_c \nabla^2 c + \frac{\delta}{\delta c} (F_{el}/N_v) \right) \quad (15)$$

We use Allen–Cahn equation[34] for the evolution of the order parameters,

$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta}{\delta \eta_i} (F/N_v) \quad (16)$$

where L is relaxation coefficient. $\frac{\delta}{\delta \eta_i}$ represents the variational derivative with respective to η_i . Now,

$$\frac{\delta}{\delta \eta_i} (F/N_v) = \frac{\delta}{\delta \eta_i} (F_{ch}/N_v) + \frac{\delta}{\delta \eta_i} (F_{el}/N_v) \quad (17)$$

and

Download English Version:

<https://daneshyari.com/en/article/10155826>

Download Persian Version:

<https://daneshyari.com/article/10155826>

[Daneshyari.com](https://daneshyari.com)