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Effect of particle-matrix coherency on Zener pinning: A phase-field approach

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ABSTRACT

We performed two sets of phase-field modeling to investigate effect of particle-matrix coherency on Zener pinning. The accuracy of the phase-field framework was examined by comparing the simulated results of a single precipitate-grain boundary interaction with the theoretical predictions. A 3D grain growth simulations with second-phase particles of different matrix-particle coherency were performed. We evaluated how coherency of precipitates and matrix affected the grain survival duration in the system.

1. Introduction

About seventy years ago, the mechanism of Zener pinning was proposed by Zener and Smith [1]. They assumed the incoherent spherical second-phase particle with isotropic interface energy with infinite system size. In succession of Zener and Smith's great achievement, there have been intensive effort to extend a range of application of Zener and Smith's original work. The grain boundary deformation under particle-boundary interaction (hereafter PBI) in a finite system size was evaluated [2]. Also, the ellipsoidal particles [3–6] at the particular particle orientations and cylindrical particles [7] at arbitrary orientations were considered. Li and Eastering evaluated the effect of the particle eccentricity (shape factor) at arbitrary particle orientations [8]. Furthermore, effect of interface coherency is analytically estimated [8,9]. Their consistent conclusion was that a coherent second-phase particle is more effective in terms of Zener pinning rather than an incoherent second-phase particle. Since the elastic effect presents at the coherent interface, it is much challenging to consider the coherent interface in a computational approach. Due to the recent progress on the atomistic modeling capability, the effect of the particle coherency was investigated using the molecular dynamics [10,11]. The works significantly contribute to enhance the understanding of the coherent PBI, however, still their size and time scales are limited due to the expensive computing cost of the atomistic modeling. On the other hand, the interfacial coherency is treated by a simplified method in mesoscale, i.e. particle-matrix interfacial energy is not uniform. The coherent particle is rarely considered in PBI study in the mesoscale. In 2D, the effect of the interfacial energy inhomogeneity (particle coherency) with an evolving second-phase particle was investigated using the phase-field method [12]. In this study, we investigated an effect of particle coherency in PBI using the phase-field method in 3D system. We performed set of simulations of a single particle-boundary [6] and grain growth with second-phase particles [13] to enhance systematic knowledge about Zener pinning by coherent inert particles when grain boundary energy and mobility is isotropic.

2. Phase-field model of grain growth with inert second-phase particles

We adopted the multi order parameter phase-field model [14] with the implementation of the Active Parameter Tracking [15] algorithm.

$$\eta_1(\mathbf{r},t), \eta_2(\mathbf{r},t), \ldots, \eta_Q(\mathbf{r},t), \tag{1}$$

where η_i $(i = 1, 2, \ldots, Q)$ are the non-conserved order parameters representing crystallographic orientation. The total number of order parameters is Q, only P-order parameters $(P < Q)$ were only allowed to evolve [5,13]. The parameters represent the second-phase particles $(Q - P)$ are constant during the simulation.

The relaxation of the η_i is governed by the Ginzburg-Landau (Allen-Cahn) time-dependent equations,

$$\frac{\partial \eta_i(\mathbf{r},t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i(\mathbf{r},t)}, \quad i = 1, 2, \ldots, P \tag{2}$$

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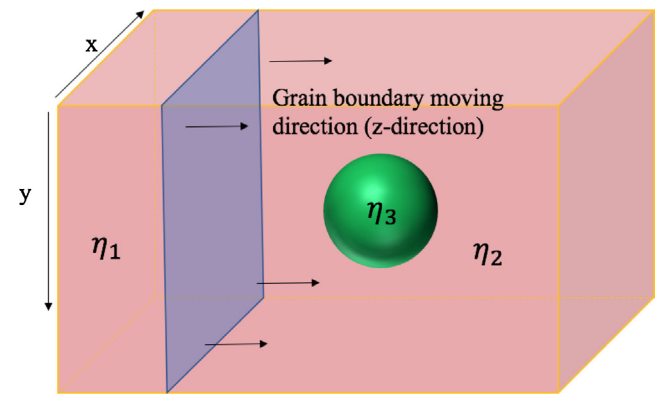

Fig. 1. Schematic drawing of initial configuration of PBI analysis. The grain indicated by η_1 expands as time goes and the grain boundary between η_1 and η_2 interacts with the inert particle η_3.

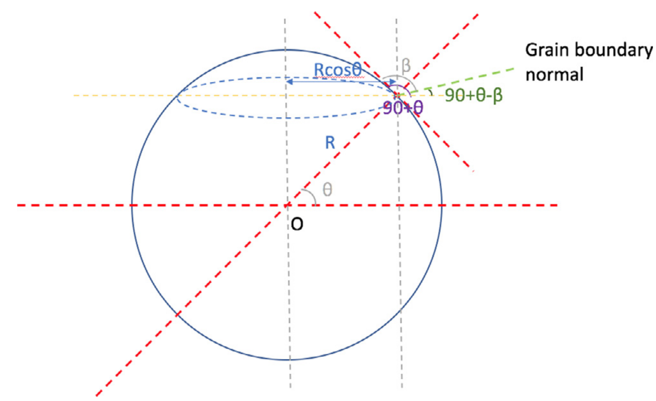

Fig. 3. Schematic drawing of spherical particle-grain boundary interaction at coherent/incoherent interface.

The total free energy function F is written as:

$$F = \int_V \left[\sum_{i=1}^{P} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \omega_{ij} \sum_{i=1}^{P} \sum_{i \neq j}^{Q} \eta_i^2 \eta_j^2 + \sum_{i=1}^{P} \left(\frac{\kappa_i}{2} \nabla \eta_i \right)^2 \right] dV. \quad (3)$$

We controlled ω_{ij} in Eq. (3) to adjust particle-matrix coherency [16,17].

We substitute Eq. (3) into Eq. (2) to obtain

$$\frac{\partial \eta_i(\mathbf{r}, t)}{\partial t} = -L_i \left(-\eta_i + \eta_i^3 + 2\omega_{ij} \eta_i \sum_{i \neq j}^{Q} \eta_j^2 - \kappa_i \nabla^2 \eta_i \right), \quad i = 1, 2, \ldots, P. \quad (4)$$

3. Phase-field model of particle/grain boundary interaction

PBI was analyzed withe incoherent interface was performed in Ref. [6]. We modified the driving force term to maintain the equilibrium order parameter value 1.0 as follows:

$$F = \int_V \left[\sum_{i=1}^{2} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \omega_{ij} \sum_{i=1}^{2} \sum_{j \neq i}^{3} \eta_i^2 \eta_j^2 + \sum_{i=1}^{2} \left(\frac{\kappa_i}{2} \nabla \eta_i \right)^2 + \zeta \times \left(\frac{\eta_2^3}{3} - \frac{\eta_2^2}{2} \right) \right] dV. \quad (5)$$

The initial configuration of the system is schematically drawn in Fig. 1.

The system cell size is $256\Delta x \times 256\Delta y \times 256\Delta z$. $\kappa_i = 1.0$ and $\Delta x = \Delta y = \Delta z = 1.0$ and $\Delta t = 0.1$. The periodic boundary condition

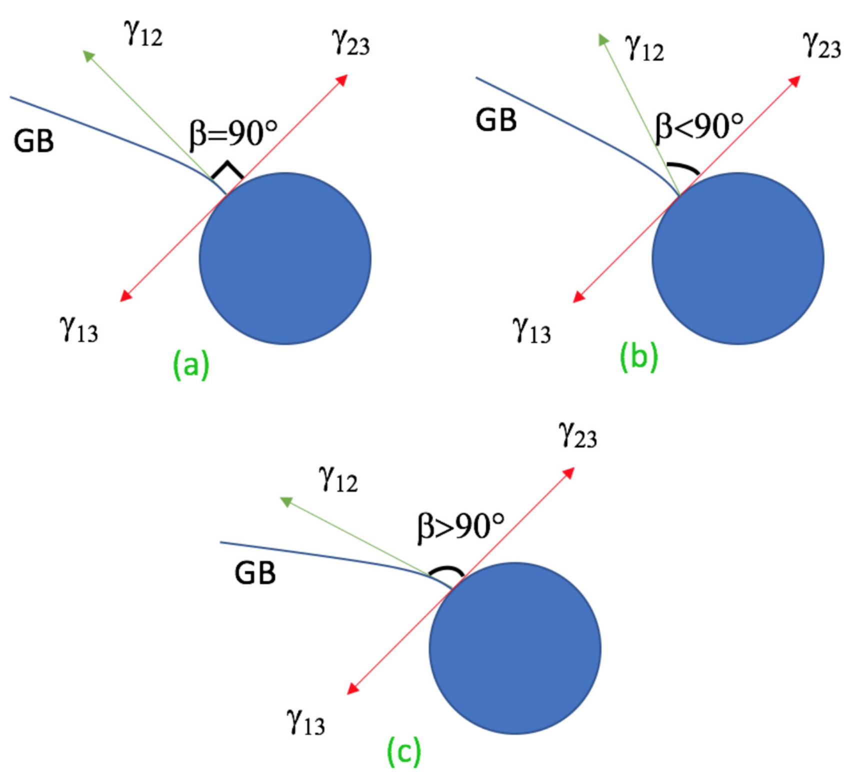

Fig. 2. (a) Incoherent particle-matrix interface. ($\gamma_{23} = \gamma_{13}$ and $\beta = 90^\circ$). (b) Coherent particle-matrix interface. ($\gamma_{13} > \gamma_{23}$ and $\beta > 90^\circ$). (c) Coherent particle-matrix interface. ($\gamma_{13} < \gamma_{23}$ and $\beta < 90^\circ$).