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Pinning force from multiple second-phase particles in grain growth

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ABSTRACT

A factor that can reduce particle pinning force significantly in grain growth is found when the grain-boundary is pinned by multiple particles. The pinning force, in this case, is a function of particle radius over inter-particle distance. A previously proposed phase-field model for particle pinning is used to validate this predicted pinning force reduction in two and three dimensions. When applied to coherent pinning particles, the same effect is observed in simulations. It is shown that, at application relevant high particle volume fraction, the average grain size is affected by this reduction of pinning force.

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1. Introduction

Study of the particle pinning in grain growth has been an important topic for a long time since introducing second-phase precipitates is one of the most commonly used method to inhibit grain growth and achieve better mechanical properties through Hall–Petch relation in polycrystalline materials. The pinning force, as formulated by Zener, comes from grain-boundary (GB) which forms a bow-out toward the migration direction during its interaction with a second-phase particle [1]. Therefore, the GB shape near the pinning particle is critical to pinning force evaluation [2,3]. When multiple particles are considered, the total pinning pressure is assessed using a summation of pinning force from individual particles [4–6]. While both experimental and computational studies have shown good agreements with this theory, they also suggested a deviation from the prediction at high particle volume fraction [5]. Different corrections have been proposed in this case based on the break-down of random particle distribution [10,12], particle overlaps [20] or the so called Louat effect where the pulling force of particles in front of an advancing boundary is considered [7,8]. However, an important factor, the change of near-particle GB shape at high particle volume fraction has been ignored.

In this work, we address this issue by calculating the GB shape between nearby particles exploiting a previously ignored factor in Ashby's work [2], and demonstrate, using both analytics and numerical method, how the change of GB shape reduces the pinning force and affects the average grain size at high particle volume fraction.

2. Particle pinning force in grain growth

In a configuration where two pinning particles are close to each other (which occurs at high volume fraction, or in low volume fraction case with highly inhomogeneous distribution of second-phase particles), the GB shape needs be determined using Ashby's method [2] since the near-particle boundary shape in Hellman's approach [3] is only a zero driving force approximation. The axi-symmetric curvature equation for a single particle in cylindrical coordinates is a second order ordinary differential equation (ODE) with driving force P as a free parameter [2].

$$\frac{z_R}{R}\frac{1}{\sqrt{1+z_R^2}}+\frac{z_{RR}}{(1+z_R^2)^{3/2}}=\frac{P}{\gamma}. \tag{1}$$

Here γ is the GB energy, R and z are defined in Fig. 1, z_R and z_{RR} are the 1st and 2nd derivative of z with respect to R. Ashby et al. solved this equation by integrating from the GB-particle contact point with a given position angle β (as defined in Fig. 1) and an interface balance condition $\cos\alpha=(\gamma_1-\gamma_2)/\gamma$ where γ_1 is the surface energy for particle-grain1 interface, γ_2 is the surface energy for particle-grain2 interface [2]. These two boundary conditions specify the coordinates and the GB slope at the contact point. With a prescribed driving force P, GB energy γ and two particle-grain interfacial energies γ_1 and γ_2, the GB shape is completely determined by solving Eq. (1). However, Ashby imposed another condition that requires a flat boundary at the midway ($L/2$) of

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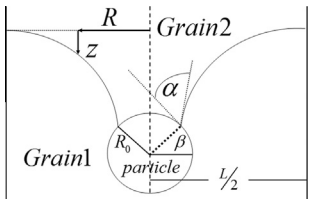

Fig. 1. A boundary seperating grain1 (lower grain) and grain2 (upper grain) is pinned by multiple second-phase particles of radius R_0 and inter-particle distance L. Only one pinning particle is shown in this window of size L to demonstrate the geometry, other nearby particles are located at distance L from this one. Window boundary lines (the two vertical solid lines) are drawn exactly at the mid-point of two adjacent pinning particles. The GB surface is a function of (R, Z) coordinates. Position angle β gives the GB-particle contact point. Angle α which is defined between GB line and the particle surface tangent is given by Young's force balancing condition. Surface energies are not labeled here. A modification angle α is needed due to particle coherency. For an incoherent particle, $\alpha = \pi/2$ since $\gamma_1 = \gamma_2$. For a coherent particle, $\alpha < \pi/2$.

two particles, and argued that such a condition gave a relationship between driving force P and angle β (note: this is an L dependent relation). This argument seems reasonable but is inconsistent with their theory on the critical pinning angle presented earlier in the same paper [2] as we will see.

The pinning force in Fig. 1 configuration is simply $F_z = 2\pi R_0\gamma\cos\beta\cos(\alpha-\beta)$. The maximum pinning force is then $F_z^{\max} = \pi R_0\gamma(1+\cos\alpha)$ with the critical pinning angle given by $\beta^{\text{crit}} = \alpha/2$. However, according to Ashby's flat midpoint argument, the angle β^{crit} should be associated with the maximum driving force $P^{\max}$ with inter-particle distance L as a parameter. For $\beta > \beta^{\text{crit}}$, a stable pinning configuration can exist only under a decreased driving force $P < P^{\max}$. Now, it is easy to see an inconsistency between the two β^{crit} relations since one depends on the inter-particle distance L while the other is a simple function of α. To resolve this controversy, the maximum pinning force will be derived analytically in two dimensions (2D) with the inter-particle distance L as a parameter, and generalized to three dimensions (3D) numerically.

2.1. Pinning theory in 2D

While the particle pinning theory in 2D is very different from its 3D cousin, it is a simpler demonstration of the basic physics. We choose to present our L dependent pinning force theory in 2D first because our key argument can be presented analytically in this case. In 2D, Fig. 1 is still a good illustration of the basic geometry. Instead of solving for 3D GB shape from Eq. (1), the 2D GB shape is a simple circle with radius ρ given by $\rho = \gamma/P$. The flat midpoint condition can be easily expressed as the following:

$$\frac{L}{2} = R_0\cos\beta + \frac{\gamma}{P}\cos(\alpha-\beta). \tag{2}$$

This configuration is stable as long as the driving force is smaller than $P^{\max}$ beyond which the grain-boundary will detach from the pinning particle. One can see that the condition for maximum driving force is $\sin(\alpha-\beta) = 2\sin\alpha R_0/L$ by rearranging Eq. (2) and using $\partial P/\partial\beta = 0$. Since the pinning force is given by $2\gamma\cos(\alpha-\beta)$, by eliminating the cosine factor with the maximum driving force condition, the maximum pinning force is then:

$$F_z^{\max} = 2\gamma\sqrt{1-\left(\frac{2R_0}{L}\right)^2\sin^2\alpha}. \tag{3}$$

For incoherent particles, the maximum pinning force is reached at $\beta = \cos^{-1}(2R_0/L)$ rather than the simple 2D maximum pinning force condition $\beta = \pi/2$. Comparing with the classic pinning force theory that gives $F_z^{\max} = 2\gamma$, this equation indicates that particle pinning becomes less effective when the inter-particle distance becomes comparable with the particle size. Although derived in 2D, Eq. (3) clearly demonstrates that the maximum pinning force is given by not only the local contact condition (angle α) but also the relative size of particle over inter-particle distance.

2.2. Pinning theory in 3D

To formulate the same L-dependent particle pinning theory in 3D, one needs to solve for the GB shape from Eq. (1) numerically (we use simple 4th order Runge–Kutta). Integration of the curvature equation (Eq. (1)) starts from the midway ($L/2$) with flat boundary condition $dz/dR = 0$ and $z = C_1$. On the other end, the GB should join the pinning particle at the correct angle such that the surface energy balance condition $\cos\alpha = (\gamma_1-\gamma_2)/\gamma$ is satisfied. Assuming a spherical particle of radius R_0 is centered at the origin, this joining angle condition can be expressed as:

$$\left.\frac{dz}{dR}\right|_{R=R_0\cos\beta} = \cot(\alpha-\beta). \tag{4}$$

By tuning the initial condition C_1, the GB line can be moved up and down such that the point with correct joining angle can be positioned on the particle sphere. The maximum driving force $P^{\max}$ and the associated position angle $\beta^{\max}$ are then found by increasing P continuously until there is no correct solution for the GB shape. Since the pinning force is given by $F_z = 2\pi R_0\gamma\cos\beta\cos(\alpha-\beta)$, the maximum pinning force can be directly evaluated with $\beta^{\max}$.

In the regime where the particle radius is much smaller than the inter-particle distance, we found that the GB-particle joining angle $\beta^{\max}$ for the maximum pinning force configuration is actually very close to the critical value $\beta^{\text{crit}} = \alpha/2$. This is expected as this condition is very similar to the single particle configuration Ashby used to derive the relation. As the inter-particle distance becomes comparable to the particle size, $\beta^{\max}$ becomes smaller than β^{crit}. Solution of GB shape for $\beta = \beta^{\text{crit}}$ in this condition still exists but only for a smaller driving force P and is not dynamically accessible by surface energy minimization in the phase-field method we use to validate the theory in the next section.

3. PF model for quantitative evaluation of particle pinning force

To validate the pinning force theory proposed in the previous section numerically, we employ a phase-field (PF) model to evaluate the particle pinning force. As demonstrated in previous works [9,19], this method can quantitatively reproduce the particle pinning force at single particle level in grain growth. Here the model is briefly described and more details can be found in Ref. [9]. The phase-field free energy functional is:

$$F = \int\left[f_0(\eta_1,\eta_2,\eta_3) + \frac{1}{2}\sum_{i=1}^{2}\xi_i K(\nabla\eta_i)^2 + Ph(\eta_1,\eta_2,\eta_3)\right]dv, \tag{5}$$

where the gradient energy coefficient is a product of numerical parameter ξ_i and dimensional constant K, and

$$f_0 = \Delta f\left[a\sum_{i=1}^{2}\left(-\frac{\eta_i^2}{2}+\frac{\eta_i^4}{4}\right) + \sum_{i=1}^{3}\sum_{j<i}c_{ij}\eta_i^2\eta_j^2 + b\prod_{i=1}^{3}\eta_i^2\right], \tag{6}$$

with dimensional constant Δf, numerical parameter a, b and c_{ij}. Here, the first two terms are commonly seen in PF grain growth model, while the last term in f_0 is added to account for the triple junction. A P term coupled with function $h = -\eta_1^3(10-15\eta_1+6\eta_1^2)$ is also added to account for the grain growth driving force in this two-grain-one-particle simple geometry. The simple grain growth in Fig. 1 is modeled with η_1 for grain1, η_2 for grain2 and η_3 for pinning

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