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Theoretical and numerical investigations on grain boundary migration due to inverse pinning

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ABSTRACT

Theoretical and numerical investigations are carried out into the inverse pinning effect of platelet particles on the grain boundary migration. The theoretical expression for the driving force of the inverse pinning proposed in an early work is first revisited and modified to remove the limitation in the volume fraction of the particles. In addition, it is shown that there exists the maximum velocity of the grain boundary due to the inverse pinning. The validity of the present considerations is demonstrated by phase-field simulations for the grain growth.

1. Introduction

Utilization of second phase particles in controlling grain structures of polycrystalline materials is one of the important techniques, the essential ingredient of which is the physics of the particle–boundaries interaction. It has been widely acknowledged that the existence of the particles causes retardation of the grain boundary migration during the grain growth processes. There have been a number of theoretical, experimental and simulation studies on this aspect, i.e., the pinning effect [1–10]. On the other hand, as exemplified by the case of AlN particles in steels [11], the particles with the anisotropic interfacial energy can induce and accelerate the migration of grain boundaries. Nishizawa called this phenomenon "inverse pinning" [11].

In contrast to the usual pinning effect, little has been clarified for the inverse pinning effect. It is often the case that interface properties between the matrix and second phase particle exhibit a strong anisotropy and, in this respect, the inverse pinning effect is considered as one of the effects often emerging in material production processes. This effect was recently investigated by phase-field simulations for the grain growth and it was found that it is highly possible that the inverse pinning causes the abnormal grain growth [12]. Hence, it is important to elucidate the detail of the inverse pinning effect, especially its kinetics.

Nishizawa proposed that the driving force for the inverse pinning of platelet particles $\Delta G_{\mathrm{inv}}(\mathrm{J\,m^{-3}})$ can be approximated by the following equation [11]:

$$\Delta G_{\mathrm{inv}} = \frac{2 v_{\mathrm{m}} f_{\mathrm{v}}}{w_{\mathrm{p}}}(\sigma_2 - \sigma_1), \tag{1}$$

where v_{m} is the molar volume of the matrix, f_{v} is the volume fraction of the particle, w_{p} is the thickness of the platelet particles and $\sigma_1(\sigma_2)$ is the interfacial energy between the particle and grain 1 (grain 2). When $\sigma_2 > \sigma_1$, the boundary migrates due to ΔG_{inv}, yielding the growth of grain 1 and the shrink of grain 2. It should be pointed out that the detailed exposition was not given for the derivation of Eq. (1) in Ref. [11] and several important points remain to be analyzed and elucidated especially regarding the validity and application range of this equation. Although the validity of this relation was demonstrated for some cases by phase-field simulations [12], a more detailed and systematic investigation is required for deeper understanding of this effect and its practical utilization in material production processes. As will be shown later, Eq. (1) is validated for the system with small volume fraction of platelet particles. Therefore, it is not applicable to systems with relatively high volume fraction of the particles.

In this paper, Eq. (1) is first re-derived and modified to eliminate the limitation of the small volume fraction. Then, the kinetics of the inverse pinning is analyzed, which elucidates the maximum velocity of the grain boundary moving due to the inverse pinning. Finally, the validity of these discussions is investigated by phase-field simulations.

2. Driving force of inverse pinning

The driving force of the inverse pinning ΔG_{inv} given by Eq. (1) is first reexamined. ΔG_{inv} is now expressed as $\Delta G_{\mathrm{inv}} = v_{\mathrm{m}}\Delta P_{\mathrm{inv}}$ with the inverse pinning pressure ΔP_{inv}. For the sake of expedience,

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we shall consider the bi-crystalline material where the grains 1 and 2 are separately by the grain boundary normal to y direction and the platelet particles are regularly-arrayed periodically in x direction. The length (y-direction) and width (z-direction) of each platelet particle are assumed infinitely large compared with the thickness, w_p (x-direction). A part of this system is schematically shown in Fig. 1a where L_x corresponds to a distance between the platelet particles periodically arraying in x-direction. The interfacial energy between the particle and the grain 1 (grain 2) is denoted by $\sigma_1(\sigma_2)$. When the grain boundary moves the distance of Δy in $+y$ direction, the resulting change of the total energy amounts to $2\Delta y L_z(\sigma_2 - \sigma_1)$. Hence, the energy change per the moved length, which corresponds to the inverse pinning force, is given by $2L_z(\sigma_2 - \sigma_1)$. The pressure exerting on the grain boundary, viz., the inverse pinning pressure is then obtained by dividing the inverse pinning force by the area of the grain boundary. When the particle thickness w_p is small compared with L_x, i.e., f_v is small, the area of the grain boundary can be approximated by L_zL_x. Then the pinning pressure is given by $\Delta P_{inv} = 2(\sigma_2 - \sigma_1)/L_x$. Since the volume fraction of the particle is $f_v = w_p/L_x$, one can obtain $\Delta P_{inv} = 2(f_v/w_p)(\sigma_2 - \sigma_1)$. The substitution of this relation into $\Delta G_{inv} = \upsilon_m \Delta P_{inv}$ yields Eq. (1).

As discussed above, Eq. (1) is considered applicable to the systems with the small volume fraction of particles, because the area of the grain boundary is approximated by L_xL_z in its derivation. This limitation can be readily removed as follow. When w_p is not sufficiently small, the area of the grain boundary is not L_xL_z but $(L_x - w_p)L_z$, as understood from Fig. 1a. Hence, the inverse pinning pressure is given by $\Delta P_{inv} = 2L_z(\sigma_2 - \sigma_1)/((L_x - w_p)L_z) = 2(\sigma_1 - \sigma_2)/(L_x - w_p)$. Using the relation $1/L_x = f_v/w_p$, the pinning pressure is rewritten as $\Delta P_{inv} = 2f_v(\sigma_2 - \sigma_1)/(w_p(1 - f_v))$. Hence, the driving force is given as

$$\Delta G_{inv} = \upsilon_m \Delta P_{inv} = \frac{2\upsilon_m}{w_p}\left(\frac{f_v}{1-f_v}\right)(\sigma_2 - \sigma_1). \tag{2}$$

In contrast to Eq. (1), ΔG_{inv} in Eq. (2) is not proportional to f_v. This correction becomes important when f_v is high. It is noted that Eq. (2) is reduced to Eq. (1) when f_v approaches null.

The most important fact understood from Eqs. (1) and (2) is that the driving force of the inverse pinning is proportional to the difference between the interfacial energies, i.e., $\Delta\sigma = \sigma_2 - \sigma_1$. However, the maximum value actually exists in the driving force, above which the driving force is independent of $\Delta\sigma$. In order to make this point clear, we re-derive Eq. (2) on the basis of the curvature of the grain boundary. It is generally accepted that the migration velocity of a segment of the grain boundary is proportional to the pressure difference caused by its local curvature [2]. This pressure is given by σ_g/r with the local curvature radius of the boundary r and the grain boundary energy σ_g. The inverse pinning pressure ΔP_{inv} can be derived from this relation by taking into account the change of the curvature radius due to the particle–boundary interaction. In the inverse pinning phenomenon, the grain boundary is generally curved near the triple junction because of the energy balance between σ_1, σ_2 and σ_g. The two-dimensional image of the inverse pinning process is depicted in Fig. 1b where θ is the angle between y-axis and the grain boundary at the triple junction. If the shape of the whole grain boundary can be approximated by the segment of a single circle, its curvature radius r is described by $r = d/(2\cos\theta)$. Here, d is the thickness of the grain and it can be expressed in terms of f_v and w_p as $d = w_p(1 - f_v)/f_v$. Hence, by substituting these relations into $\Delta P_{inv} = \sigma_g/r$, the following equation for ΔG_{inv} is obtained,

$$\Delta G_{inv} = \frac{2\upsilon_m\sigma_g}{w_p}\left(\frac{f_v}{1-f_v}\right)\cos\theta. \tag{3}$$

Here $\cos\theta$ is given as $\cos\ \theta = (\sigma_2 - \sigma_1)/\sigma_g$, provided that the shape of the boundary at the triple junction takes the equilibrium shape according to Young's law. Therefore, Eq. (3) is completely equivalent to Eq. (2). However, the form of Eq. (3) explicitly presents an important fact that the upper limit exists in ΔG_{inv}. The upper limit is realized when $\cos\theta = 1$. This condition corresponds to the complete wetting of the interface between the grain 1 and the particle by the grain 2.

Now, our focus is directed at the migration of the grain boundary due to the inverse pinning. The migration velocity of the grain boundary due to the inverse pinning V_g is given by using ΔP_{inv} as follows,

$$V_g = m\Delta P_{inv} = m\sigma_g\frac{2}{w_p}\left(\frac{f_v}{1-f_v}\right)\cos\theta = 2\ \cos\theta V_{ref}, \tag{4}$$

where m is the grain boundary mobility and

$$V_{ref} = m\sigma_g\frac{1}{w_p}\left(\frac{f_v}{1-f_v}\right) = \frac{m\sigma_g}{d}. \tag{5}$$

As already described above, $d(= w_p(1 - f_v)/f_v)$ is the thickness of the grain 2. V_{ref} is called the reference velocity in this paper and it can be regarded as the velocity of the boundary in the system without the effect of the particle as will be discussed in Section 4. It is important to mention that the migration velocity of the grain boundary due to the inverse pinning is proportional to the reference velocity. The proportionality coefficient is entirely determined by the balance between the interfacial energies and the grain boundary energy. When the proportionality coefficient is maximum, viz.,

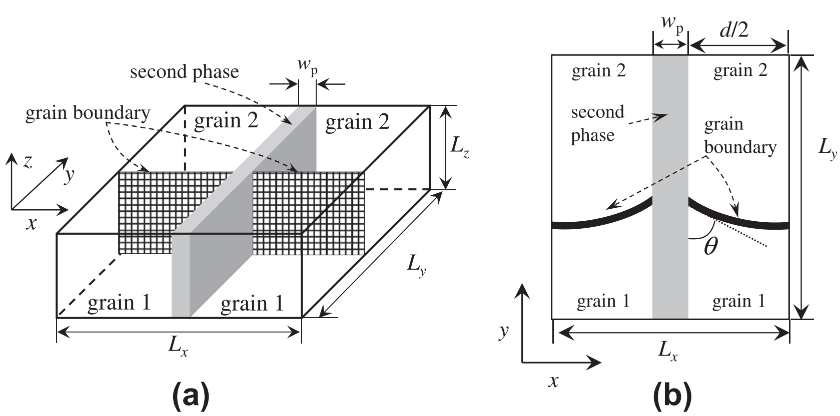

Fig. 1. (a) Three-dimensional and (b) two-dimensional illustrations of the inverse pinning process.