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# Two modes of grain boundary pinning by coherent precipitates

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## ABSTRACT

We propose a two-mechanism theory to estimate the pinning effect of coherent precipitates on grain-boundary (GB) migration in grain growth, taking into account the important effect of elastic misfit strain at the coherent interface. Depending on the relative importance of the elastic and the GB contributions to the total free energy, Zener type stabilization or a novel elastic energy induced stabilization may occur. It is found that the pinning is most effective in the crossover region between these two mechanisms. A phase-field-crystal model is used to numerically validate the theory. Relevant experiments and potential impacts on alloy design are also discussed.

## 1. Introduction

Second-phase precipitates formed in alloy microstructure strengthen materials by blocking dislocation motion or stopping grain growth at elevated temperature and therefore limiting the propagation of plastic deformation [1–3]. There have been extensive studies on the interactions between precipitates and GBs in order to understand their inhibiting effect on grain growth and improve materials strength [4–8]. Precipitates can generally be separated into two types: coherent and incoherent. For coherent precipitates within a given grain, the lattice planes across the interfaces between the precipitates and grain matrix are continuous, and the lattice parameter differences between the precipitates and matrix are accommodated by elastic strains. Therefore, coherent interfaces have relatively small interfacial energy, but they generate strain energy. For incoherent precipitates, the lattice planes for the precipitates and matrix grain terminate at their interfaces. Incoherent interfaces generally possess higher interfacial energy while the shear strain energy is relaxed.

Although coherent precipitates have long been believed to be effective pinning units for GB migration, the role of the elastic strain in GB pinning has not yet been fully understood. Existing investigations have been largely focused on the interactions between incoherent precipitates and GBs in limiting grain growth [2,5,6,9] described by Zener's theory which takes into account only the interfacial energy contributions in pinning [10,11]. Pinning force from coherent particles has been calculated based on Zener's theory. It is shown that, by only considering interfacial energies, coherent particles are more effective in pinning GB migration. The classic continuum elasticity theory works well for describing the dislocation-coherent particle interactions. However, it is a challenge to generalize it to describing the GB-coherent particle interactions due to the fact that a segment of the coherent particle-matrix interface loses its coherency when a GB replaces it during the migration, partially relaxing the elastic energy. The change of interface coherency in turn modifies the stress distribution along the remaining coherent part of the interface and affects the GB migration near the particle.

To reveal the interaction mechanisms between a GB and a coherent interface during the GB migration generally requires a sophisticated computational approach at the continuum level. To avoid the complication introduced by the moving GB and the change of interface property, we propose a qualitative theory to estimate the effect of misfit generated elastic energy on the GB migration based on energy competition criterion using a simplified interface geometry. The phase-field-crystal model (PFC) which naturally captures the effect of elasticity and the change of

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interface coherency, and operates at grain growth related long time scale, is then used to examine the atomistic interaction mechanisms between a migrating GB and a coherent particle.

## 2. Theory

The particle pinning theory in grain growth, as formulated by Zener, is based on the balance of interfacial energies at the contact point [2]. When a second-phase particle intersects with a moving GB, it forms a new interface with the growing grain, replacing the original interface with the shrinking grain. The GB-particle contact point in 2-dimension (2D) or the contact line in 3-dimension (3D) becomes a triple junction (line). The line tensions from the two particle-grain interfaces and the GB need to balance each other along the tangential direction of the particle-grain interface for the configuration to be stable. Since the GB motion from the growing grain to the shrinking grain is driven by the macroscopic curvature effect (the grain size is usually much larger than the second-phase particle), stable configuration of the GB in this case is a bow-out shown in Fig. 1 [12]. For a system with large grain size, the driving force for the GB motion from the grain curvature is generally small, and the curved configuration of the GB near the particle can generate enough pinning force to stop the GB migration. At smaller grain size, the curved GB around the particle is subject to a larger driving force from increased grain curvature and may not be able to entirely pin the GB migration.

One can write this process as a minimization problem based on a free energy functional. In the simple two-grain case shown in Fig. 1, it is

$$F_0 = \sum_i l_i \gamma_i + \int \Delta\mu dv + \int f_{el} dv \qquad (1)$$

where $dv$ is volume element, $\gamma$ is interfacial energy, $l$ is interface length (in 2D), the summation subscript $i$ covers the GB and the two particle-grain interfaces, $f_{el}$ is the elastic energy density, $\Delta\mu = \alpha\gamma_{GB}/D$ is the chemical potential difference for atoms across the grain boundary. It is proportional to the GB energy ($\gamma_{GB}$) over the grain diameter ($D$) with the proportional constant $\alpha$ related to grain shape. The minimization of $F_0$ is then constrained by the line tension balance condition tangential to the particle-matrix interface. Many previous computational works on particle pinning have been using this energy minimization approach without considering the elastic energy contribution [13,14]. When there is no driving force for grain growth, the total energy $F_0$ with elastic contribution is then $F_0 = 2\pi R\gamma + B\pi R^2\delta^2$ where $R$ is the 2D particle radius, $\delta$ is the particle-matrix lattice misfit, and $B$ is a constant proportional the elastic modulus of the system. To arrive at this formula from Eq. (1), we only include a single particle-matrix interface. The elastic energy expression is based on the Eshelby's inclusion theory [15]. It has been known that the total energy $F_0$ can be minimized for two limiting cases. Given a constant $\delta$, precipitates with small radius form coherently in the matrix since the added elastic contribution is smaller than the cost of switching the particle-matrix interface from low energy coherent configuration to high energy incoherent one. On the other hand, since the elastic contribution ($\sim R^2$) will eventually dominate over the interfacial energy contribution as the radius grows; large precipitates then form a high energy incoherent interface with the matrix to relax the elastic strain energy. This competing elastic strain energy and interfacial energy also explain the commonly observed phenomenon of precipitate coherency loss after swept by a GB. For a typical metal system with GB energy $\gamma \sim 1J/m^2$ lattice misfit $\delta \sim 5\%$ and elastic modulus $B \sim 100GPa$, the elastic energy $B\pi R^2\delta^2$ will surpasses the interfacial energy $2\pi R\gamma$ when the particle size is on the order of 10 nm. It also suggests that, if the elastic energy is small, precipitates would energetically prefer to form a coherent interface with the new host grain [16–18].

Similar to the steady-state energy argument discussed above, we can estimate the driving force for the grain boundary migration. To extend the Zener pinning theory which only considered interfacial energies, we also include the contribution of elastic strain energy to the pinning effect of coherent precipitates. If the elastic energy contribution is much larger than the interfacial energy, the evolution of interface configuration is then mainly driven by the minimization of $(\Delta\mu + f_{el})$. By wrapping the GB around the particle, the total elastic energy can be significantly decreased from the coherency loss at the interface while the only price paid is the increase of the total GB energy due to elongated GB length which is less significant in this limit. An interface geometry similar to the Zener pinning is then formed (Fig. 2c). It is expected that the largest elastic energy density appears near the coherent interface. Therefore, in addition to the Zener surface tension balance condition, the GB migration near the particle

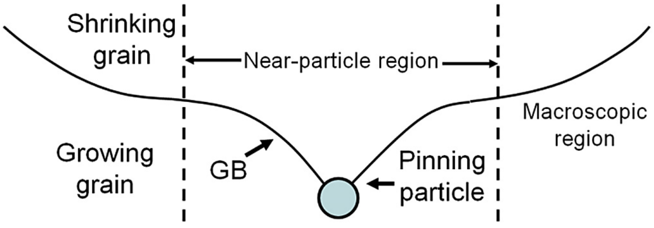

**Fig. 1.** A schematic showing the Zener particle pinning geometry. Far away from the pinning particle (macroscopic region), the GB has a curvature given by the grain size. Near the particle, the GB changes significantly from the shape in the macroscopic region and forms a bow-out configuration.

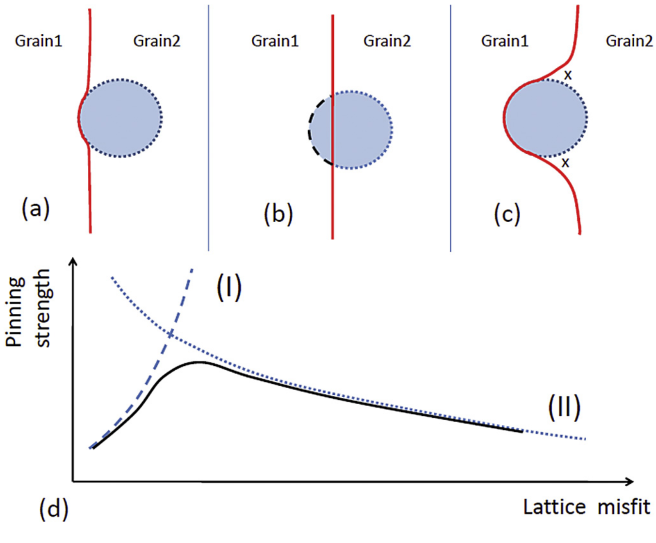

**Fig. 2.** Illustration of the particle-GB interaction and the pinning strength of coherent precipitates. The GB is migrating from the left to the right. Red solid line is the GB/incoherent interface. Blue dotted line is the original coherent interface the particle formed with grain 2. The small elastic energy case is shown in (a). To further migrate GB from (a), a new coherent interface with grain 1 (black dashed line) can form as shown in (b). The large elastic energy case is shown in (c) with high elastic energy density region marked by "x". A possible crossover behavior is demonstrated in (d) where the dashed line (I) is based on the small elastic energy case and the dotted line (II) is based on the large elastic energy case, the result pinning strength is shown as the solid line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)