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Phase-field study of zener drag and pinning of cylindrical particles in polycrystalline materials

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ABSTRACT

Zener drag and pinning in composites reinforced with cylindrical particles is investigated using three-dimensional phase-field simulations. Detailed systematic studies clarify the effect of relative orientation of the particle and length/diameter ratio on the kinetics of drag. It is shown that a combination of local equilibrium at junctions in contact with the particles, initial driving force of the migrating grain boundaries, and configuration of the particles within the polycrystalline matrix determine the intensity and persistence of drag and pinning effects.

1. Introduction

Today industrial materials are in need of excellent physical, chemical and processing properties that are obtained by combining prominent properties of two or more pure substances to fulfill requirements in endless applications [1,2]. The excellent mechanical, electrical and thermal properties of added materials, such as carbon nanotubes [3–5], promise stronger reinforced composites with better functional properties. The microstructure evolution of such composites is of fundamental and technological interest [6–8]. The grain growth resistance in metal matrix composites is well-investigated for secondary particles of spherical and ellipsoidal shapes [9–12], while the behaviour of deviating shapes is still poorly understood. Here, we focus on the effect of particles with large length/diameter ratio, resembling cylinders which are less investigated in the literature but largely used in composite materials.

Previous investigations of particle drag and pinning are mostly concerned with randomly distributed particles with spherical [9,10,13], ellipsoidal [11,12], and cubic shapes [14]. Cylindrical particles have some properties of both spherical and cubic particles with a much larger length/diameter ratio. It is, for instance, application-relevant to know whether longer cylinders have an advantage over shorter ones and if orientation plays a role in the pinning of grain boundaries. Furthermore, in composite materials the strengthening particles are usually distributed non-randomly due to the production process.

Theoretical studies on the shape of particles suggest an increase of maximum pinning force F with deviation from spherical shape, depending on the orientation [15]. Ryum and coworkers [12] studied an ellipsoidal particle with a–a–b axes and the shape factor $\varepsilon = b/a$. The moving interface is assumed to be aligned parallel to the a–a plane of the ellipsoid (case 1) or parallel to the a–b plane (case 2):

$$F_{Sphere} = \pi\sigma R, \tag{1}$$

$$\text{Case 1:}\ F_{Ellipsoid} = F_{Sphere}\,\frac{2\varepsilon^{-1/3}}{(1+\varepsilon)}, \tag{2}$$

$$\text{Case 2:}\ F_{Ellipsoid} = F_{Sphere}\,\varepsilon^{0.47}, \tag{3}$$

$$F_{Cube} \approx 1.45\,F_{Sphere} \tag{4}$$

with R the radius of the sphere and σ the grain boundary energy. The force of an ellipsoidal particle at constant volume depends on its orientation with respect to the grain boundary. Cuboidal particles have a higher pinning force as long as $\varepsilon < 0.619$ for case 1 and $\varepsilon < 2.204$ for case 2. The overall drag effect, however, depends not

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only on the pinning force, which is a static measurement of maximum area reduction, but also on the kinetics of the migrating grain boundary and the dynamics of interaction. Moreover, within a polycrystalline body, particles can sit in various locations and also have a cooperative impact on the network of grain boundaries. These aspects can be studied using simulation methods which can consider any geometry of particles and resemble the dynamics of moving boundaries as well as equilibria at the junctions in a physically sound picture.

The aim of the current work is to study Zener drag and pinning of cylindrical particles embedded in polycrystalline materials using the multi-phase-field method [16], which allows studying simultaneous evolution of grain boundaries and junctions next to the particles. We first investigate interaction with a single grain boundary and the effect of orientation, driving force, and formation of triple junctions. Later we study drag and pinning for particles sitting in different positions in the grain boundary network, and the cooperative drag effects in a polycrystalline body. Finally, we discuss pinning of cylinders of different length in polycrystalline bodies.

2. Multi-phase field model and simulation details

The multi-phase-field approach [16–18] applies to studying two or more phases (or grains) in contact where the phase-field variables are constrained to

$$\sum_{\alpha=1}^{N}\phi_\alpha = 1, \tag{5}$$

where $\phi_\alpha \in [0,1]$ and N is the number of existing domains. Previous studies have shown the ability of this method to reconstruct junctions at the equilibrium [19,20] and to study grain growth in polycrystalline materials [21,22]. The multi-phase field model starts with the total free energy functional F_{total} over a given domain Ω:

$$F_{total} = \int_\Omega \left(f^{GB} + f^{CH} + f^{EL} + \ldots\right)\mathrm{d}V, \tag{6}$$

where f^{GB} is the interfacial free energy density, f^{CH} the chemical free energy density and f^{EL} the elastic free energy density. In the present work, the interfacial free energy density is the only contribution of interest expressed in pairs

$$f^{GB} = \sum_{\alpha=1}^{N}\sum_{\beta\neq\alpha}^{N}\frac{4\sigma_{\alpha\beta}}{\eta}\left\{-\frac{\eta^2}{\pi^2}\nabla\varphi_\alpha\cdot\nabla\varphi_\beta + \varphi_\alpha\varphi_\beta\right\}, \tag{7}$$

where η is the interface width and $\sigma_{\alpha\beta}$ is the interfacial energy between domains α and β. The temporal evolution of the phase-field variables follows [23].

$$\dot{\varphi}_\alpha = -\sum_{\beta=1}^{N}\frac{\mu_{\alpha\beta}}{N}\left(\frac{\delta}{\delta\varphi_\alpha} - \frac{\delta}{\delta\varphi_\beta}\right)F_{total}, \tag{8}$$

where $\mu_{\alpha\beta}$ is the interfacial mobility. Using Equations (6)–(8) we obtain

$$\dot{\varphi}_\alpha = \sum_{\beta\neq\alpha}^{N}\frac{\mu_{\alpha\beta}}{N}\left\{\sigma_{\alpha\beta}(I_\alpha - I_\beta) + \sum_{\gamma\neq\alpha,\beta}^{N}(\sigma_{\beta\gamma} - \sigma_{\alpha\gamma})I_\gamma\right\}, \tag{9}$$

in which the generalized curvature term is given by $I_\alpha = \nabla^2\phi_\alpha + \frac{\pi^2}{\eta^2}\phi_\alpha$.

2.1. Simulation procedure

For all simulations the same physical dimensions are chosen. Common light-metal interfacial energy $\sigma_{\alpha\beta}$ and mobility $\mu_{\alpha\beta}$ are taken as 0.32 $\mathrm{Jm^{-2}}$ and 3×10^{-16} $\mathrm{m^4J^{-1}s^{-1}}$ [24], respectively. The interfacial energies between all phases and grains are the same. Time step dt and grid spacing Δx are 1 s and 10^{-9} m, respectively. The width of the interface is benchmarked and selected as $\eta = 7\Delta x$ to guarantee high accuracy and reasonable computation time. The size of the simulation box depends on the type of investigation: for studying drag of a single cylinder we use a box size of 180^3 and $150^2 \times 250$ grid cells, and for studying polycrystalline composites we use a box size of 512^3 grid cells. The cylinder radius is 7.5 nm and the maximum cylinder length is 100 nm. It is well-known that particles can break during manufacturing processes, e.g., ball-milling before sintering, which results in shorter particles which are investigated here. Particles are arranged both randomly and ordered in direction and position, and the contact between them is prohibited.

For a systematic investigation of anisotropic interaction, we performed simulations with different orientations between the particle and a flat grain boundary driven by an artificial driving force $\Delta G_{\alpha\beta}$. This driving force adds to the kinetic Equation (9) for $\dot{\phi}_\alpha$ as $\mu_{\alpha\beta}h(\phi_\alpha)\Delta G_{\alpha\beta}$. Thus, the velocity of the flat interface between grain α and β is given as

$$v = \frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial\phi_\alpha}{\partial t}\frac{\partial x}{\partial\phi_\alpha} = \mu_{\alpha\beta}\frac{\partial x}{\partial\phi_\alpha}h(\phi_\alpha)\Delta G_{\alpha\beta}. \tag{10}$$

In order to have a simple linear relationship between v and $\Delta G_{\alpha\beta}$, we have chosen $h(\phi_\alpha) = \partial\phi_\alpha/\partial x$. For the double obstacle potential used in our model

$$h(\phi_\alpha) = \frac{\partial\phi_\alpha}{\partial x} = \frac{\pi}{\eta}\sqrt{\phi_\alpha\phi_\beta} \tag{11}$$

and thus $v = \mu_{\alpha\beta}\Delta G_{\alpha\beta}$.

For numerical stability, the driving force should be restricted to $\Delta G_{\alpha\beta} < 2\pi\sigma/\eta$ [25]. Note that if, for example, the interface is moving towards grain β (α is growing), $\frac{1}{2}\mu_{\alpha\beta}h(\phi_\alpha)\Delta G_{\alpha\beta}$ is added to $\dot{\phi}_\alpha$ and $-\frac{1}{2}\mu_{\alpha\beta}h(\phi_\alpha)\Delta G_{\alpha\beta}$ to $\dot{\phi}_\beta$. To ensure the stability of the cylinder particles as an inert phase, related interfacial mobility is reduced by a factor of 10^{-25} compared to boundaries between grains.

3. Results and discussion

3.1. Effect of orientation and grain boundary kinetics on the drag

Cylindrical particles are expected to have an orientation-dependent Zener effect, similar to that of ellipsoidal [15] and cubic particles [14]. Here, we analyse the interaction between a moving boundary and a cylindrical particle with different orientation angles. We measure the in-contact boundary velocity, which is the distance travelled by the grain boundary while being in contact with the cylinder divided by the time of interaction between boundary and cylinder. Thus, we are able to discuss not only the drag effect but also the dynamics of the grain boundary depending on its driving force during the interaction. For a cylindrical particle, there is one degree of freedom for the contact angle with respect to a flat grain boundary, as shown in Fig. 1a.

The results show that the drag effect depends on the particle orientation mainly when $\theta < 45°$ (Fig. 1b and c). At low driving forces (Fig. 1b) for $\theta < 20°$ and at high driving forces (Fig. 1c) for $\theta < 8°$, the in-contact velocity significantly drops and particle drag becomes more efficient than a spherical particle of the same