Kinetics of particle drag and pinning; Phase-field modelling and simulation

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Abstract

Multi-phase field modeling and simulation has been applied to investigate the kinetics of grain boundary influenced by particle drag and pinning. For different grain boundaries of different velocities, three kinds of interactions have been characterized. Full pinning is found to occur below a certain driving force namely the pinning force. Increasing the driving force, pinning effect is less pronounced and the mobility converges to a constant value. The mobility in this case is below the theoretical value of an unloaded grain boundary and depends on fraction volume of particles. The large scale grain growth simulations also have been performed for spherical particles and the grain size distribution has been investigated.

The effect of shape of the particles has also been considered in the interaction with a flat interface. The results show the interfacial mobility is highly affected with the shape of particles. A linear dependency between V, mobility, and R, shape factor inverse, is found. This is consistent with theoretical formulation of shape-dependent pinning forces, driven by Ryum et al [1].

Measuring the mobility of boundary during interaction, we have found that at low driving forces it decreases exponentially till pinning happens. For higher driving force the mobility recover the linear form but it is below theoretical value for free grain boundary value. The interaction can be divided into three stages as it is described in the figure.

The pinning force however found to be lower than that of Zener's equation. The results are quite similar to simulations performed by Hazledine and Oldershaw [3].

The mobility as a function of driving force can be fitted (dash lines) nicely into an exponential form as

\[ \dot{\psi} = \mu G \exp \left( \frac{-aG}{AG - G_c} \right) - \ddot{\psi} \]

In their paper, Ryum et al. had shown that the shape of particles may significantly influence the restraining force on the grain boundary. For the case investigated here they suggest following equation for drag force:

\[ \Sigma = \frac{f}{\pi R^2} \]

To understand the effect of shape we track the interaction of a moving boundary with single particle of different shape factor (R). It has been observed that plate-like particles induce higher force on the grain boundary which result severe deformation. We consider the whole process of interaction as three stages; touching, detaching and release of interface.

Figure 10 shows the total boundary area varying during the interaction. It is clear that the kinetic of boundary is highly effected with the shape of particle. The maximum area achieved just before releasing is proportional to drag force imposed by the particle into the interface. However, it cannot represent the drag force entirely, while local curvature may have an additional contribution which is not fully covered by the total area values.

We measured the mobility for grain boundary during attachment to the particle for different cases. It is found that V is proportional to 1/R (R > 1). Figure 11 shows the 1/V versus R. Comparing with Ryum’s formulation (above mentioned) it reveals that mobility and force has direct connection.

Motivation

In previous works, it is mostly aimed to offer pinning condition based on maximum force acting on the boundaries no matter what may happens before or after contact. Therefore till today the kinetic and dynamic of interface during interaction is poorly understood.

The fact that interface deforms during interaction with the particle motivate us to consider the kinetic of interface in the presence of particles. To predict the interface mobility under drag force is one of the main goals of current study.

Another influencing factor on drag and pinning forces is the shape of particles which we considered here.

Effect of shape

In order to reconstruct reliable regulation for Zener’s model, multi-phase field (MFP) provides us the possibility to set up fully controlled conditions for the simulation. We consider a flat interface moving under a constant driving force which passes through the randomly distributed particles. More details can be found in ref [2].

Large scale grain growth in the presence of spherical particles

We had simulated grain growth for different amounts of particles; 0.0201, 0.0516 and 0.1165 volume fraction within a box of 300x300x300 with initially 5000 grains. Simulations were performed by our open source code for multi-phase field model named OpenPhase [4].

Average grain size for different cases is compared to ideal grain growth as well as each other in figure 5. It is shown that for 11.65% of particles growth is nearly pinned. For fewer amount of secondary phase (2.01% and 5.16%) the growth is slowed down by dragging but the parabolic form of growth kept valid.

Figure 6 and 7 show 3D and cross section of our simulation box for different conditions but at the same time. Color coding refer to the same grains for all cross sections. It has been observed that grain size distributions for the growth under drag (pinning) significantly deviate from ideal growth. Figure 8 shows the grain size evolution for different simulations.

As it is predicted in the literature, the peak in the distribution function shifted to the left (smaller grain size).

Conclusions

Current study demonstrates the ability of multi-phase field modelling in order to discuss drag and pinning effects on the grain growth. In summary we have found that:

• the interaction between particles and moving grain boundary can fall into different regimes which show different kinetics.
• the mobility of the boundary follows an exponential form which approaches to a constant at high driving force.
• the grain size distribution (for large scale simulations) during grain growth found to be a subject of change due to drag (pinning) effect.
• shape of the particle may affect significantly the deformation of boundaries as well as its kinetic. We had found the linear dependency between grain boundary mobility and the inverse of shape factor.

References