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Phase field simulations of grain growth in systems containing second-phase particles

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Abstract

A phase field model for grain growth in materials containing inert, immobile particles has been implemented. Large scale 2D-simulations were performed for different sizes and volume fractions of the second-phase particles and different initial grain sizes of the matrix phase. For all simulations the mean grain size and the number of particles located on grain boundaries as a function of time were determined. The agreement with Monte Carlo and front-tracking simulations is very good. From comparison with experiments suggestions for further improvement of the simulations are made.

Introduction

Many theories and simulation techniques that describe the pinning effect of particles on grain boundaries during grain growth have been developed. The main objective is to predict the limiting mean grain size $\overline{R}_{lim}$ where further grain growth is inhibited by the particles. Nevertheless, there are still small but essential differences between theories, simulations and experiments that are not completely understood. The purpose of our research is dual, firstly to understand which parameters determine the interaction between grain boundaries and particles, and secondly to incorporate them appropriately in a phase field model. The present paper mainly deals with large scale 2D-simulations.

Phase field model and implementation

For a complete description of the model we refer to [1]. The polycrystalline microstructure of the matrix phase is represented by a set of phase field variables $\eta_1(\mathbf{r},t), \eta_2(\mathbf{r},t), \ldots, \eta_p(\mathbf{r},t)$. The evolution of the $\eta_i(\mathbf{r},t)$ is obtained from

$$\frac{\partial \eta_i}{\partial t} = -L_i \left[m \left(-\eta_i + \eta_i^3 + 2\eta_i \sum_{j \neq i}^{p} \eta_j^2 + 2\eta_i \Phi \right) - \kappa_i \nabla^2 \eta_i \right] \quad (1)$$

for $i = 1, 2, \ldots, p$. L_i are kinetic coefficients related to the grain boundary mobility, κ_i are the energy gradient coefficients, $\mathbf{r}$ is the position vector and t is time. Φ is a spatially varying parameter that equals 1 inside the particles and 0 elsewhere. m is related to the depth of the free energy well.

For all simulations $p = 36$, $m = 1$, $\kappa_i = 0.5$ and $L_i = 1$, giving isotropic grain boundary properties with a grain boundary energy equal to 0.40 J/(grid point) [1]. Nearly spherical particles with radius $r = 2.5$ and $r = 3$ are used. The area fraction of the particles f_a ranges between 0.002 and 0.16 and the position is randomly chosen. For the numerical solution of (1) a semi-implicit Fourier-spectral method is used with $\Delta x = 1$ and $\Delta t = 1$. System size is 256x256 or 512x512 grid points (g.p.). To initialize the microstructure, small random values between -0.001 and 0.001 are assigned to the phase field variables. Then, the microstructure is allowed to evolve according to (1) with $\Phi = 0$ until a mean grain size $\overline{R}_0$ is reached. $\overline{R}_0 = 0$ refers to simulations where particles are immediately included.

MATLAB is used for the implementation and simulations are performed on a IBM Pseries 630 with power4 processors of 1GHz and 4 GB RAM. For systems of 256x256 g.p., 30 hours are required for 60000 time steps. In the case of 512x512 g.p. this takes more than 10 days and the memory requirements are close to the maximum available.

Large-scale 2D-simulations

The following relation between $\overline{R}_{lim}$, $\overline{r}$ and f_a is often assumed

$$\frac{\overline{R}_{lim}}{\overline{r}} = \frac{b}{f_a^{\beta}} \quad (2)$$

where b and β depend on the grain boundary geometry at a particle intersection.

Figure 1 gives the $\overline{R}_{lim}/r$-values obtained from 2D phase field simulations. Especially for low volume fractions the number of particles and the number of grains in the limiting microstructure is rather low. As a consequence, there is a considerable scatter on the results and the mean over a large number of simulations should be taken to obtain a reliable value for $\overline{R}_{lim}$.

The phase field results for $\overline{R}_0 = 0$ give $b = 1.38$ and $\beta = 0.46$. In [1] we showed that due to the diffuse interfaces the pinning force of a particle is slightly too high. This might

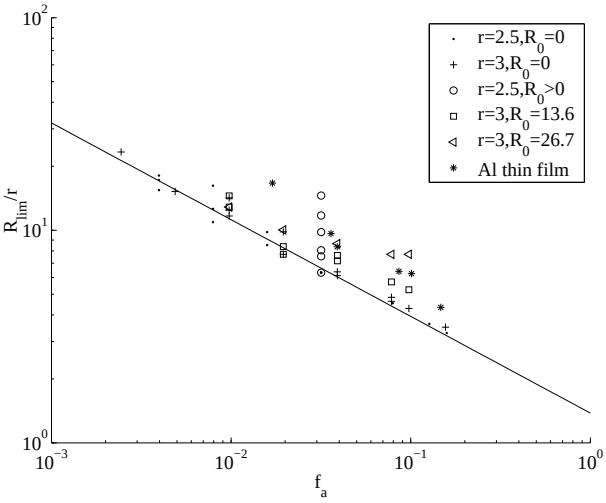

Figure 1: $\overline{R}_{lim}/r$ as a function of f_a obtained from phase field simulations compared with experimental results for thin Al-films containing $CuAl_2$-particles. ($\circ$ correspond to data points for $r = 2.5$, and $\overline{R}_0 = 0, 10.6, 13.7, 13.8, 25.5$ and 34.0, from bottom to top.)

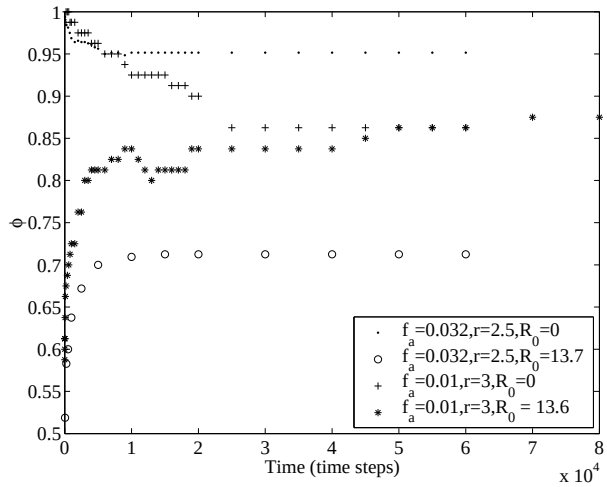

Figure 2: Evolution of ϕ during grain growth for different $\overline{R}_0$ and different f_a.

influence the value of b, but has no effect on β. Our results agree quite well with 2D Monte Carlo ($b = 1.2, \beta = 0.55$ [2]) and front-tracking ($\beta = 0.46$ [3]) simulations.

The simulations for $\overline{R}_0 > 0$ show that (2) is not always true, as $\overline{R}_{lim}$ might as well depend on $\overline{R}_0$. To understand the role of the initial grain size, in figure 2 the temporal evolution of ϕ is shown for different $\overline{R}_0$ and different f_a. For $\overline{R}_0 = 0$, particles are present during the nucleation of the microstructure and therefore the grain boundary configuration is highly correlated to the position of the particles ($\phi \approx 1$). During grain growth, boundaries escape from some of the particles and ϕ decreases slightly. For $\overline{R}_0 > 0$, initially the grain boundary configuration is random and the number of particles contributing to the pinning effect is smaller than for $\overline{R}_0 = 0$ ($\phi \ll 1$). During grain growth, the moving grain boundaries are pinned by the particles they meet. As a consequence, ϕ increases in time, however often $\overline{R} > \overline{R}_{lim}$ (with $\overline{R}_{lim}$ from (2)) before the number of grain boundary/particle intersections is high enough to cease grain growth. Only for very low f_a and $\overline{R}_0$ not too large, $\overline{R}_{lim}$ is not affected by the initial microstructure.

In figure 1, the experimental data points for thin Al-films containing $CuAl_2$-particles [4] are above the relation we obtained for $\overline{R}_0 = 0$. A first explanation is that in the Al-films many particles were located within grains ($\phi < 1$) reducing the pinning effect of the particle distribution. However, there are many more parameters that influence the pinning effect of particles on grain boundaries. There are for example the characteristics of the particle interface (coherent or incoherent), the orientation dependence of the grain boundary energy and mobility and the stability of the particles. In 2D the orientation dependence of the surface energy and the drag-effect from surface grooving at grain boundaries are also important.

Concluding remark

The presented model agrees very well with theory and other simulation techniques as most of them do not consider the properties of the particles and the particle interface. However, for comparison with real systems, more parameters and phase field variables should be included into the model and parameters should allow dependence on the phase field variables. This will make the simulations even more computationally intensive. Further, more experimental information on the properties of the particles, grain boundaries and particle interfaces, but also a dynamic description of the movement of a grain boundary through a particle are required to improve the simulations.

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