Grain Growth Simulations Including Particle Pinning Using the Multiphase-field Concept

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In this paper, the effect of particle pinning on grain boundary motion is investigated by phase-field modeling. In general, the kinetics of grain growth in multicrystalline materials is determined by the interplay of curvature driven grain boundary motion and the balance of interfacial tension at the vertices of a grain boundary network. A comprehensive way to treat both effects in one model is given by the phase-field approach. The specific feature of the multiphase-field model used for this investigation is its ability to treat each grain or phase boundary with its individual characteristics, together with a thermodynamic coupling which allows a sound treatment of phase transformation, e.g. the formation of precipitates of a second phase.

The pinning effect itself is simulated on the nanometer scale resolving the interaction of individual inert or reactive precipitates with a curved grain boundary. From these simulations an effective pinning force is deduced, and a model for a driving force dependent grain boundary mobility is formulated accounting for the pinning effect in the grain growth simulation on the mesoscopic scale. These simulations demonstrate how particle pinning leads to much slower growth kinetics and a different grain morphology with higher boundary curvatures in the stationary state. Finally, an increase of the pinning force due to a changing particle density, e.g. during heat treatment, is shown to result in a transition between normal and abnormal grain growth before grain coarsening is inhibited completely.

KEY WORDS: phase-field; particle pinning; abnormal grain growth; inert particles; NbC particles.

1. Introduction

The simulation of grain growth is one of the earliest applications of phase-field type models in the field of materials science. An early example is the work of Allen and Cahn1) where they developed a model for the evolution of anti-phase boundaries. This model describes the movement of interfaces driven solely by interfacial curvature and is able to model ideal grain growth of an ideal and homogeneous material. However, the modeling of real materials requires various extensions. Crystalline materials obey a certain crystallographic symmetry which result in interfacial properties which are far from being constant, but depend e.g. on the lattice mismatch and therefore on the crystal lattice orientation relationship of neighboring grains. Also, the interaction of interfaces with inclusions or solute atoms requires more degrees of freedom in the model to take into account the various effects. These issues were addressed by a variety of phase-field models in the last decade.2–6)

In technical applications, pinning is used to control the grain size of a material during heat treatment. A common example is microalloyed steel with Nb, Ti or Al as alloying elements. Nb, e.g. will form NbC-precipitates and size, density and spatial distribution of these precipitates are important factors which can be used to limit the grain size during heat treatment, especially in the high temperature austenitic phase. Because the NbC-precipitates can only be considered as inert and stable particles in a limited range of process parameter, it is important to take into account particle formation and dissolution if technical applications are addressed.

In this paper we will briefly sketch a general multiphase-field model7,8) and discuss its application for simulating grain growth and particle pinning in solids. The model allows to assign separate properties like interfacial energy and mobility to each dual interface between grains or phases. Results of simulations performed on the length scale of individual inert or reactive particles will be presented. In a further step, an effective interface mobility function is derived from the simulations which is then applied to describe particle pinning in grain growth simulations on the mesoscopic scale of a polycrystalline grain structure.

2. The Multiphase-field Model

The phase-field concept naturally considers interfacial curvature, and no conceptual difficulties appear when switching from a 2D to a 3D implementation. Furthermore, the phase-field concept allows an integrative treatment of grain growth driven by interfacial curvature, together with phase transformations.
In the following we will give a brief overview of the multiphase-field model which was used for the simulations reviewed in this paper. In the multiphase-field model each individual grain is described by its own phase-field variable $\phi_i$. In general, we consider a system of $N+1$ field variables $\phi_i, i=0, \ldots, N$. These variables can be identified with the local phase state (liquid, solid matrix, precipitate) and with individual grains of a solid phase identified by their lattice orientation. In the bulk of grain $i$, $\phi_i=1$ holds, on grain boundaries between grain $i$ and grain $j$, $\phi_i+\phi_j=1$. In general, the constraint $\sum_{i=0}^N \phi_i=1$ is fulfilled everywhere. The model dates back to the work,\(^7\) and a recent formulation is described in Ref. \(^9\).

The free energy functional $F$ for this system is now expanded to a sum over all pairwise energy differences between two grains $i$ and $j$

\[
F = \int_V \sum_{i,j=1}^N f_{ij}^{\text{int}}(\phi_i, \nabla \phi) + f_{\text{chem}} dV \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots 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radius of 220 nm, to grain growth simulations on a larger scale without resolving the particles anymore.

In Fig. 1, snapshots of a grain boundary moving through a random arrangement of inert particles are shown. The boundary is moving from the top to the bottom. The coloring of the boundary represents the local curvature of the $\phi=0.5$ isoplane. The local bending around the particles is clearly visible.

The simulations are based on the following material data: isotropic grain boundary and particle–matrix interfacial energies $\mu_{ij}=1 \cdot 10^{-5} \text{J/cm}^2$ for all interfaces. Interfacial mobility $\mu_{ij}=5 \cdot 10^{-3} \text{cm}^3/\text{s}$ for the grain boundary, the mobilities of the particle–matrix interfaces are set 10 orders of magnitude smaller to keep the particle inert and suppress any particle–matrix interface movement. A constant thermodynamic force $\Delta G$ between the grains is applied in the phase-field simulation to drive the grain boundary. It may represent a mesoscopic curvature of the grain boundary (beyond the microscopic scale) or a loaded state due to deformation.

For a cubic particle arrangement, the simulation domain can be restricted to one unit cell of the particle array. In this case, the variation of the critical pinning force with the particle density was derived from the phase-field simulations and compared to the Zener model which considers a cubic arrangement as well. The average grain boundary velocity is plotted against the applied driving force $\Delta G$ for different particle volume fractions $f_V$ (Fig. 2).

The grain boundary starts to pass the obstacles at driving forces above the critical value for the driving force $p^*$ and approaches the linear dependency with the velocity proportional to $\Delta G$ asymptotically for high values of $\Delta G$. Within numerical errors the calculated values of $p^*$ are in good agreement with the Zener pinning pressure according to Eq. (5). The calculated velocities follow the velocity function

$$v(\Delta G) = \mu \Delta G \exp\left(\frac{-\alpha p^*}{\Delta G - p^*}\right) \quad \text{where} \quad \alpha \approx 0.12$$

with a constant $\alpha$ adjusted to 0.12 to fit uniquely all calculations independent of the driving force $\Delta G$. The exponential function (6) is motivated by the notion, that the detachment of the boundary from the particle may be described like the overcoming of an energy barrier. From Eq. (6) one can derive a description for the effective grain boundary mobility $\mu(\Delta G)$:

$$\mu = \mu_0 \exp\left(\frac{-\alpha p^*}{|\Delta G| - p^*}\right)$$

for $|\Delta G| > p^*$. $\mu = \mu_{\text{min}} \ll \mu_0$ else ...(7)

A finite mobility $\mu_{\text{min}}$ is defined for driving forces below the critical pinning pressure. This is mainly for numerical convenience in order to maintain the diffuse interface profile. Equation (7) replaces the constant mobility $\mu$ in Eq. (4). Beside the thermodynamic driving force the curvature pressure is calculated separately and the sum of both values enter the mobility function.

In the case of an irregular particle distribution, the number of simulated arrangements may not be sufficient to draw a firm conclusion, but, compared to a cubic arrangement, the grain boundary velocity is reduced. This is an indication, that an irregular structure shows enhanced particle drag caused by a larger positive contribution of dense regions to the overall pinning compared to the negative effect of dilute regions.

3.2. Active Particles

As active particles we understand precipitates, e.g. carbides, which can change their volume or shape on the time scale under consideration. NbC precipitates were treated as an example for a coupled phase-field simulation which combines grain growth and particle precipitation. As could be shown in the case of inert particles, size, density and distribution of precipitates govern the pinning force. Therefore, model descriptions of these quantities as a function of time and space are necessary for a comprehensive understanding of the particle pinning effects.

Compared to inert particles, the treatment of active particles requires higher numerical effort because diffusion has to be considered in the whole simulation domain. This can be a severe challenge on microscopic scale due to numerical time step criteria when solving the equations explicitly. A further problem is the almost stoichiometric composition of carbide particles with high C and Nb content compared to the Fe-matrix: For low matrix concentrations, large simulation domains with high resolution are required to allow...
the growth of several particles. However, 2D simulations can be performed on single CPU computers and results will be shown below.

Phase-field simulations were performed for the austenitic phase in an Fe–C–Nb steel, using direct coupling to thermodynamic databases for the calculation of the driving pressure acting on the NbC/austenite interface. For the thermodynamic description, the TCFE3 database\cite{12} was used. The grain boundary energy was set to $\gamma = 1 \cdot 10^{-5}$ J/cm². The diffusion coefficient of Nb in austenite is $1.8 \cdot 10^{-12}$ cm²/s, C diffusion is set to infinity in austenite, justified by the small considered volume. Nb and C diffusion in the NbC-particle is neglected. Calculations were done for isothermal conditions at a temperature of 1 300 K.

In Fig. 3, a sequence of pictures show the interaction between a single NbC particle with a moving grain boundary. At the initial stage, a single particle with an initial radius $r = 20$ nm is set in a matrix with a Nb concentration close to the equilibrium value of $[\text{Nb}] = 0.004$ at%. For the concentration field, periodic boundary conditions are applied. The grain boundary is allowed to maintain arbitrary angles at the simulation domain boundary. The movement of the grain boundary is only driven by interfacial curvature, no additional thermodynamic driving force was applied. The graph in Fig. 4 displays the evolution of the average matrix concentration of Nb as a function of time for three configurations: an individual particle, a particle interacting with a grain boundary and a particle attached at a grain boundary triple junction. The initial particle sizes are identical in all cases. Once the grain boundary touches the particle the local surface curvature is changed due to the force balance at the new triple junction. The Nb concentration reacts directly on the moving particle-matrix interface. The grain boundary moves towards its stable position within $\approx 50$ s. The equilibrium shape of the particle is obtained on a time scale which is a factor of 10–100 longer, because it involves not only the grain boundary motion but also Nb diffusion which is the rate limiting process under these conditions.

The curves in Fig. 4 show that the final concentration of dissolved Nb in the matrix depends on the configuration. The isolated particle leads to the highest Nb concentration which compensates the curvature undercooling. When the particle is located within a grain boundary its shape is modified. The average surface curvature is decreased when it takes an ellipsoidal shape instead of a sphere. This causes a smaller curvature undercooling and the solubility decrease. Although the effect is small, under certain conditions it may lead to a favored precipitation at grain boundaries which will then lead to a non uniform particle distribution.

Figure 5 shows results from a many-particle simulation for the same conditions described above. Now, 18 individual NbC-precipitates with radii between $r = 15$ nm and $r = 30$ nm are set at the beginning. An initially curved grain boundary evolves into a final configuration of straight sections between individual NbC particles. On the time scale of this simulation, Ostwald ripening of the NbC precipitates does not change the number of precipitates, however the different Nb concentration around the particles represent a driving force for further ripening. This requires mass trans-

![Fig. 3. Interaction of one NbC particle with a grain boundary, domain size is 0.1×0.1 μm², Δx=1 nm, η=6Δx. The picture pairs denote the Nb-concentration field (left) and the position of the interface (right) after 2 s, 8 s, 3 200 s and 6 400 s of ripening. In the interface map 0 means bulk phase, 1 dual interface and 3 triple junction. Note that the former spherical NbC particle transforms into an elliptical shape.](image)

![Fig. 4. Change of the average Nb concentration in the Fe-matrix.](image)

![Fig. 5. Many-particle simulation after 100 s (left) and 10 h (right) of ripening. The domain size is 0.6×0.6 μm³ (600×600 grid points, η=6Δx). A grain boundary is pinned within an array of NbC-precipitates. The colors denote the Nb concentration showing local differences caused by different particle radii.](image)
port between the particles which is retarded by the small diffusivity of the Nb atoms. Because the Nb matrix concentration with respect to the particle does not only depend on the particle radius, but also on the location of the particle, a situation of inverse ripening may occur in which small precipitates, located on grain boundaries or triple junctions will grow on the cost of larger particles located in the matrix.

4. Scale Bridging

4.1. Grain Growth Simulation with Particle Pinning

The effective mobility function (7), deduced by direct simulation on the microscopic scale, is used to simulate the pinning effect on the mesoscopic scale on a 250 \( \mu \text{m} \times 250 \mu \text{m} \) grid, where the particles themselves cannot be resolved anymore. The initial grain structure was generated by a weighted Voronoi construction using 290 grains. As material data we used \( \mu_0=5 \cdot 10^{-3} \text{cm}^3/\text{s} \) and \( \sigma=1 \cdot 10^{-4} \text{J/cm}^2 \).

To avoid numerical problems in the limit \( \mu \to 0 \), a minimum mobility \( \mu_{\text{min}}=0.01 \mu_0 \) was introduced. Starting from an initial grain structure with an average grain radius of 8.4 \( \mu \text{m} \), the grain growth of the matrix grains driven by reduction of interfacial area was calculated (Fig. 6) with and without particle pinning. The particle concentration was chosen as 0.22% corresponding to a critical pinning pressure \( p^* = 0.03 \text{J/cm}^2 \). To overcome this barrier in 2D a grain boundary curvature \( \kappa=p^*/\sigma \) is necessary. This value corresponds to a mean grain radius of \( \langle r \rangle = 33 \mu \text{m} \) in the 2D simulations.

After a first period of fast growth and vanishing of small grains, the average grain radius increases slowly and tends to stabilize below 15 \( \mu \text{m} \). This is by a factor of 2 below the critical grain size calculated from the Zener pinning pressure. This deviation is tentatively attributed to topological constraints of the grain boundary network which did not show high grain boundary curvatures anymore, but further investigations are necessary to verify this. The growth behavior of the drag free grain growth can be fitted with a growth exponent of 0.5, i.e. \( \langle r \rangle \sim \langle r \rangle^{1/2} \) (Fig. 7). For particle drag the radius increase follows an exponent of about 1/10 for the simulation with \( p^* \geq 0.03 \text{J/cm}^3 \). However, the fitted curve shows systematic deviations, because the structure tends to a stable configuration with \( \langle r \rangle = \text{const} \) which does not follow a simple power law scaling. The exponent in the first stage of the grain coarsening depends on the critical pinning force. To quantify this dependency needs further investigation. Another interesting feature of the grain growth simulation is, that even in the final grain structure the majority of the grain boundaries show a significant curvature. This is clearly due to the pinning model and a clear distinction to simulations without pinning, where all grain boundaries tend to form straight lines.

4.2. Abnormal Grain Growth

A further example demonstrates the appearance of abnormal grain growth dependent on the pinning parameter and the initial grain size. Characteristic for abnormal grain growth is the rapid growth of relatively few grains in an otherwise unchanged structure. This phenomenon which degrades the mechanical properties is often observed in microalloyed case hardening steels. The prevention of abnormal grain growth is an important goal during the production of case hardening components. Two parameters, the pinning force and the initial distribution of the grain sizes, i.e. conglomerations of small grains, determine whether abnormal grain growth occurs or not. Using the effective mobility approach it is possible to investigate the microstructure evolution depending on these variables. In a series of simulations for a variation of the pinning forces between 0 and 0.08 J/cm$^2$ and different initial grain sizes, normal, abnormal and no grain growth could be observed, Fig. 8. In this figure, the parameter range for abnormal grain growth is shaded. The lower and upper limits mark the area of abnormal grain growth between the parameter ranges of normal and no grain growth.
The critical line in the middle of the abnormal growth regime reflects the most dangerous combination of initial austenite grain diameter and pinning force which leads to the appearance of huge grains in the microstructure. However, the distinction between normal and abnormal grain growth can not be defined by a simple criterion and in this study the calculated grain structures are sorted into the different groups by visual inspection. Therefore, the transition can not be fixed to a certain value, but the morphology map in Fig. 8 indicates the parameter range where abnormal grain growth is likely to appear.

5. Summary and Conclusion

A general multiphase-field model was applied to study different aspects of particle pinning. At first, the effect of particle drag on grain boundary motion and the effect of the boundary interaction on the particle growth was investigated on the length scale of individual particles. A main outcome of this work is the formulation of a drag force model, consistent to the Zener model, which describes the effective grain boundary mobility as a function of the applied drag force, particle size and concentration. Using simulation results obtained on the microscopic length scale of the particles, the effective drag force were derived and used to simulate grain growth on a coarser scale. Ensembles of some hundreds of grains can be treated in 2D or in 3D which allows efficient investigations of the pinning effect on the grain coarsening. The results confirm smaller growth coefficients compared to the classical \( r^{1/2} \) behavior. The growth coefficient depends on the drag force and therefore on the particle density in the material. Moreover, first simulations indicate that the average grain size of the final grain structure is significantly smaller than the critical grain size calculated from the critical pinning force of the Zener model. Dependent on the initial grain size and the pinning force, also abnormal grain growth were observed before complete pinning is achieved.

Simulations with active particles are still hindered by longer computation times compared to simulations for inert particles. Nevertheless, qualitative effects could be demonstrated: At first, the time scale of the particle–grain boundary interaction is much shorter then the shape change of the precipitates, therefore, for a wide range of applications the particles can be treated as inert for mesoscopic particle pinning simulations. In general, the matrix concentration of dissolved atoms reacts immediately on the particle–grain boundary interaction. This can change the ripening behavior of particle ensembles and one can think about conditions, when small particles located on a grain boundary can promote the dissolution of larger bulk precipitates.

The phase-field method is now capable to address various items concerning particle pinning, on the microscopic as well on the mesoscopic scale, e.g. effects of particle shape, density, and spatial distribution on the pinning force and on particle drag. It offers the possibility to treat the problem of diffusion controlled particle growth in a grain boundary network and to study precipitation at grain boundaries.

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