The Roles of Grain Boundary Energy Anisotropy and Second–Phase Particles on Grain Growth in Polycrystalline Materials

Mohsen Asle Zaeem*, Haitham El Kadiri, Mark F. Horstemeyer, Paul T. Wang
Center for Advanced Vehicular Systems, Mississippi State University
Starkville, MS 39759, USA
*mohsen@cavs.msstate.edu, +1 662-325-0126

ABSTRACT

A phase-field model was developed to investigate the concurrent effects of grain boundary energy anisotropy and second-phase particles on grain growth in polycrystalline materials. The phase-field model was developed based on the evolution of non-conserved phase-field variables according to the time-dependent Ginzburg-Landau (TDGL) equation. The Read-Shockley and modified Read-Shockley models for cubic crystals were considered to include anisotropic grain boundary energies for low and high misorientation angles between adjacent grains. Systems without particles reach a steady state grain growth rate. The presence of particles significantly alters the microstructures during grain growth. Results show that for systems with particles, the critical average grain size to stop grain growth depends on both the volume fraction and size of particles and also on the grain boundary energy anisotropy.

Keywords: Phase-field model, Grain growth, Anisotropic grain boundary energy, Second-phase particles, Finite element.

1. INTRODUCTION

Grain growth is one of the most common microstructural evolutions resulting from different materials processing [1]. Size and shape of grain microstructures determine the mechanical and material properties of alloys [2], and conducting research in this area to predict and control the microstructures at different thermal and mechanical conditions is necessary for design optimization of engineering structures. There have been several numerical studies in this area based on different computational approaches such as Monte Carlo [3,4], and phase field [5,6] methods. Most of the current models consider only a single phase for the polycrystalline material and do not include the effects of second-phase particles. Also the effect of anisotropic grain boundary energy which can significantly change the kinetics of the microstructural evolution has not been included in the numerical models of grain growth. In this research, a phase-field – finite element model is used to simulate the microstructural evolutions during grain growth considering the simultaneous effects of anisotropic grain boundary energy and second-phase particles on the growth rate.

2. FORMULATION

The polycrystalline microstructure can be described by many non-conserved phase-field variables or order parameters \( \eta_i(r,t), i = 1,2,\ldots,n \), where \( n \) is number of different orientations) [5]. These phase-field variables are continuous functions in time and space dimensions and represent different orientations for different grains (see Fig. 1). The value of the field variables varies between 0 and 1; for example for grains having the \( q \)th orientation: \( \eta_{izq}(r,t) = 1 \) and \( \eta_{izq}(r,t) = 0 \) and this transition from 0 to 1 in the grain boundaries is smooth. The total grain boundary energy of a microstructure is a function of these phase-field variables and their gradients:

\[
F = \int \left[ f(\eta_1, \eta_2, \ldots, \eta_n) + \sum_{i=1}^{n} \frac{\kappa_i}{2} (\nabla \eta_i)^2 \right] dV, \tag{1}
\]

where \( \kappa_i \) are the gradient energy coefficients. The local free energy density, \( f \), has this form:

\[
f(\eta_1, \eta_2, \ldots, \eta_n) = \sum_{i=1}^{n} \left( \frac{\alpha}{2} (\eta_i)^2 + \frac{\beta}{4} (\eta_i)^4 \right) + \gamma \sum_{i=1}^{n} \sum_{j=1}^{n} \eta_i^2 \eta_j^2 + \epsilon \Phi^2 \sum_{i=1}^{n} \eta_i^2, \tag{2}
\]

\( \alpha, \beta, \gamma, \) and \( \epsilon \) are phenomenological parameters, and \( \Phi = 1 \) inside a particle and \( \Phi = 0 \) in the matrix. Here \( n \) is the number of different orientations for grains while no orientations are considered for particles. When \( \Phi = 1 \), \( f \) has one minimum at all \( \eta_i \) equal to 0. In our simulations, the parameters of the model are considered...
to be constants similar to original model by Fan and Chen [5]: \( \alpha = \beta = \gamma = 1 \ (\varepsilon = \gamma ) \).

The evolution equations of non-conserved order parameters can be obtained from time-dependent Ginzburg-Landau (TDGL) [7] equation given by the following,

\[
\frac{\partial \eta_i(r,t)}{\partial t} = -L_i \frac{\delta F}{\delta \eta_i(r,t)}, \quad i = 1,2,\ldots,n ,
\]

where \( L_i \) are related to the grain boundary mobility (in this paper, \( L_i = 1 \) similar to Fan and Chen model [5]).

Fig. 1. Schematic of various crystal orientations using different orientation field variables for each grain. The solid-lines are grain boundaries.

The relationship between gradient energy coefficient and grain boundary energy, \( E(\theta_{ij}) \), [8]:

\[
\kappa_i = \kappa_j E^2(\theta_{ij}), \quad \theta_{ij} = \theta_i - \theta_j ,
\]

where \( \theta_i \) is the orientation angle of a grain with respect to a reference angle, \( \theta_{ij} \) is the angle between grains \( i \) and \( j \), and \( \kappa_j \) is considered to be a constant (in this paper, \( \kappa_j = 2 \), similar to the Fan and Chen model [5]). In our model to calculate \( \theta_{ij} \) for each grain boundary between two adjacent grains, we assumed a random orientation angle \( (\theta_j = [0 \pi]) \) corresponding to each order parameter (see Fig. 1).

The grain boundary energy considering low misorientation angles between adjacent grains \( (\theta_{ij} < 20^\circ) \) is presented by Read and Shockley (RS) [9]. The conventional form of RS model is [10]:

\[
E(\theta_{ij}) = E_0 \frac{\theta_{ij}}{\theta_m} \left( 1 - \ln \frac{\theta_{ij}}{\theta_m} \right), \quad \theta_{ij} < \theta_m ,
\]

where \( E_0 \) is a material constant and is proportional to the total density of dislocations (in our simulations \( E_0 = 1 \)), and \( \theta_m \) is the maximum misorientation angle for RS model \( (\theta_m = 20^\circ) \). For \( \theta_{ij} \geq 20^\circ \), \( E(\theta_{ij})/E_0 = 1 \), same as isotropic cases. For large misorientation angles, modified RS (MRS), is developed by Wolf [11]:

\[
E(\theta_{ij}) = E_0 \sin(2\theta_{ij}) \left( 1 - r \ln \sin(2\theta_{ij}) \right),
\]

where \( r \) is a constant and in our simulations \( r = 0.683 \) to make \( (E(\theta_{ij})/E_0)_{\max} = 1 \). More details about this model can be found at [12].

3. RESULTS

Eq. (3) was solved in a 400×400 square domain using the finite element software, COMSOL multiphysics [13]. A uniform mesh consists of 22000 triangular elements with quadratic interpolation functions are used to discretize the domain for all simulations. Time step size of iterations is \( \Delta t = 0.2 \). To simulate the polycrystalline material properly, 36 order parameters are used [5]. For all simulations, a same initial grains configuration is chosen to be a Voronoi tessellation diagram with 36 random initial orientation angles corresponding to order parameters, Fig. 2 (a). For cases including particles, particles are randomly distributed in the grains system where \( V_f \) and \( r_p \) are the volume fraction and size of particles, respectively.

In Fig. 2, microstructural evolution at \( t = 2000 \) is shown for the isotropic, Read-Shockley and modified Read-Shockley models of grain boundary energy. This figure shows that including the effects of anisotropic grain boundary energy significantly alter the microstructures.

(a) Initial condition (b) Isotropic

(c) Read-Shockley (d) Modified Read-Shockley

Fig. 2. Microstructural evolution. In (b)-(d) \( t = 2000 \).
The presence of second-phase particles slows or freezes the grain growth process and results in different microstructural configuration usually with finer grain sizes that can be accountable for different materials properties. Fig. 3 shows the average grain radius versus time of evolution in systems with inert particles. From Fig. 3, it is evident that including anisotropic grain boundary energy significantly affects the grain growth morphology. The critical average grain size to stop the grain growth depends not only on volume fraction and size of particles, as predicted by other models, but also on the grain boundary energy anisotropy.

4. CONCLUSIONS

A phase-field model was developed to study the simultaneous effects of anisotropic grain boundary energy and second-phase inert particles on grain growth kinetics. Including the effects of anisotropic grain boundary energies decreases the grain growth rate, and this decrease is more significant when the effect of high misorientation angles is considered. Results showed that the critical average grain radius to stop the grain growth is a function of the volume fraction and size of second-phase particles and also significantly depends on the grain boundary energy anisotropy for systems with low volume fraction of particles.

5. REFERENCES