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Phase field modelling of stressed grain growth: Analytical study and the effect of microstructural length scale

M. Jamshidian [a,b,*], T. Rabczuk [b,c,*]

[a] Department of Mechanical Engineering, Isfahan University of Technology, Isfahan, Iran
[b] Institute of Structural Mechanics, Bauhaus-University Weimar, Marienstrasse 15, 99423 Weimar, Germany
[c] School of Civil, Environmental and Architectural Engineering, Korea University, Seoul, South Korea

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ABSTRACT

We establish the correlation between the diffuse interface and sharp interface descriptions for stressed grain boundary migration by presenting analytical solutions for stressed migration of a circular grain boundary in a bicrystalline phase field domain. The validity and accuracy of the phase field model is investigated by comparing the phase field simulation results against analytical solutions. The phase field model can reproduce precise boundary kinetics and stress evolution provided that a thermodynamically consistent theory and proper expressions for model parameters in terms of physical material properties are employed. Quantitative phase field simulations are then employed to investigate the effect of microstructural length scale on microstructure and texture evolution by stressed grain growth in an elastically deformed polycrystalline aggregate. The simulation results reveal a transitional behaviour from normal to abnormal grain growth by increasing the microstructural length scale.

1. Introduction

Stressed grain boundary migration is a dominant factor for microstructure and texture evolution in polycrystalline thin films on substrates [1,2]. The experiments of Zhang et al. [3] on stressed grain growth in copper thin films on silicon substrates have shown that the strain energy minimizing grain boundary migration is responsible for the evolution of texture during annealing. The recent theoretical studies of Tonks et al. [4], Bhattacharyya et al. [5] and Kim et al. [6] employ the phase field modelling approach for simulations of stressed grain boundary migration in elastically deformed polycrystalline aggregates. The phase field method which is based on a diffuse interface description of grain boundary provides a great platform for simulations of microstructure and texture evolution in three-dimensional polycrystalline systems [7,8]. However, the big challenge is yet to conclude quantitative results from such simulations [9]. The validity of a quantitative phase field model is endorsed by comparison against the corresponding sharp interface model [10]. Particularly, the diffuse interface description of grain boundary is required to reproduce the same boundary kinetics as that of its sharp interface counterpart [11]. Through analytical and simulation investigations, Fan and Chen [12] and Garcke et al. [13] analyzed the validity and accuracy of the diffuse interface model for curvature-driven grain boundary migration. However, a similar investigation for stressed grain boundary migration is still missing in the literature.

Stressed grain growth has been experimentally observed at different microstructural length scales. Using transmission electron microscopy, Brandstetter et al. [14] studied the evolution of microstructure in nanocrystalline copper interconnect lines of width between 80 nm and 3000 nm. Sonnweber-Ribic et al. [2] utilized automated electron backscatter diffraction

* Corresponding authors.
E-mail addresses: mostafa.jamshidian@gmail.com, mostafa.jamshidian@uni-weimar.de (M. Jamshidian), timon.rabczuk@uni-weimar.de (T. Rabczuk).

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to study microstructure and texture evolution in copper thin films on polyimide substrates. In their study, the film thickness ranges from 0.5 µm to 10 µm and the average grain size scales with film thickness. Recently, Yogo et al. [15] performed in situ observation of abnormal grain growth in polycrystalline carbon steel samples of 2 mm thickness and 100 µm average grain diameter. In a recent study by Ciulik and Taleff [16], abnormal grain growth was used to produce millimeter-size single crystals from polycrystalline molybdenum sheets. These experimental studies provide a strong motivation to perform a quantitative investigation on the effect of microstructural length scale on stressed grain growth using phase field simulations. Such an applied theoretical investigation which is still missing in the literature could shed some light on the process of stressed grain growth in polycrystalline aggregates.

This paper is the first attempt to correlate between the diffuse interface and sharp interface descriptions for stressed grain boundary migration by presenting analytical solutions for a circular grain boundary in a bicrystalline phase field domain as a benchmark example. Phase field simulations for such a benchmark example are performed in order to evaluate the validity and accuracy of the diffuse interface model through comparison between the simulation results and the analytical solutions. Excellent agreement between the analytical solution and simulation results is obtained by employing a thermodynamically-consistent theory and proper expressions for the phase field model parameters in terms of the physical grain boundary related material properties.

As an application of the phase field model, the effect of microstructural length scale on stressed grain growth in a polycrystalline aggregate is investigated. Quantitative phase field simulations of stressed grain growth demonstrate that the microstructural length scale has a significant effect on the evolution of microstructure and texture. For small microstructural length scales, stressed grain growth is shown to be mostly at normal regime. This regime is identified by no conceivable change in texture, equiaxed grains and a log-normal grain size distribution (GSD). On the other hand, large microstructural length scales are shown to result in the rapid increase of the texture component with lower strain energy, growth of abnormal size grains and a bimodal grain size distribution as the characteristics of abnormal grain growth. For intermediate values of the microstructural length scale, a transitional behaviour between normal and abnormal grain growth is observed. Overall, increasing the microstructural length scale is illustrated to cause a transition from normal to abnormal grain growth by stressed grain boundary migration.

The plan of the present article is as follows. The multi-phase field theory of stressed grain boundary migration is briefly described in Section 2. Analytical solutions and phase field simulations for the migration of a circular grain boundary in a hypothetical bicrystalline thin film are presented, respectively, in Sections 3 and 4. In Section 5, phase field simulations of stressed grain growth in polycrystalline aggregates with different microstructural length scales are presented. The main findings of the present study are summarized in Section 6.

2. Theory

Following the modelling efforts of Tonks et al. [4] and Kim et al. [6], the phase field theory of stressed grain boundary migration in an elastically deformed polycrystalline aggregate is briefly described as follows. Throughout, we use the mathematical notation common in the modern continuum mechanics [17]. In the multi-phase field theory of Steinbach and Pezzolla [18], the phase field variable ϕ_i represents the local volume fraction of phase i with $i = 1, 2, \dots, N$. The integer N is the total number of different phases/crystal orientations in the polycrystalline aggregate $\mathcal{B}$. Following Kalidindi et al. [19] and Takaki et al. [20], we utilize the Taylor homogenization method and assume that the homogenized infinitesimal elastic strain $\bar{\mathbf{E}}$ is uniform throughout $\mathcal{B}$. Previous research on stressed grain growth has also shown that utilizing the Taylor homogenization method greatly reduces the computational cost of the phase field simulations with insignificant loss of accuracy [21]. The local free energy density can then be expressed in the separable form

$$\psi = \psi^{\phi}(\phi_1, \dots, \phi_N, \nabla\phi_1, \dots, \nabla\phi_N) + \psi^{e}(\bar{\mathbf{E}}, \phi_1, \dots, \phi_N). \tag{1}$$

Assuming isotropic grain boundary properties, the microstructural free energy density ψ^{ϕ} is given by [18]

$$\psi^{\phi} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\omega\phi_i\phi_j - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\kappa\nabla\phi_i\cdot\nabla\phi_j, \tag{2}$$

where ω and κ are the phase field model parameters. Using a thermodynamically consistent interpolation function [22], the elastic free energy density ψ^{e} is written as

$$\psi^{e} = \frac{\sum_{i=1}^{N} g(\phi_i)\psi_i^{e}}{\sum_{i=1}^{N} g(\phi_i)}, \tag{3}$$

with the smooth interpolation function $g(\phi_i) = \phi_i^2(3 - 2\phi_i)$ and the elastic strain energy of phase i given by

$$\psi_i^{e} = (1/2)\bar{\mathbf{E}} : \mathcal{C}_i[\bar{\mathbf{E}}]. \tag{4}$$

Here, $\mathcal{C}_i$ is the fourth-order elastic moduli tensor of phase i. For cubic symmetry $\mathcal{C}_i$ is identified by the three elastic constants C_{11}, C_{12} and C_{44} and the crystallographic orientation of phase i. Using standard thermodynamics arguments [17], the local Cauchy stress is given by