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Phase field modeling of ideal grain growth in a distorted microstructure

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

[a] Department of Mechanical Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran
[b] School of Civil, Environmental and Architectural Engineering, Korea University, Seoul, Republic of Korea
[c] Institute of Structural Mechanics, Bauhaus-University Weimar, Marienstrasse 15, 99423 Weimar, Germany

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ABSTRACT

In this work, we perform phase field simulations of ideal grain growth in a distorted polycrystalline aggregate. The distorted microstructure is assumed to be generated by homogenous deformation of an initially equiaxed polycrystalline aggregate. Phase field theory of curvature driven grain boundary migration under distortion is developed and the phase field kinetic relations are implemented in a numerical code based on an explicit time integration procedure. As a benchmark example, phase field simulations of the shrinkage of a distorted circular grain are performed and compared with that of an undistorted elliptical grain to validate the phase field theory and its numerical implementation and also to study the effect of distortion on the kinetics of grain boundary migration. The non-equiaxed distorted grain evolves towards an equiaxed geometry by curvature-driven boundary migration. The evolution rate towards equiaxity is proportional to the distortion magnitude. However, the distortion regardless of its magnitude has no effect on the decrease rate of the distorted grain surface area. We also investigate the evolution of a distorted polycrystalline microstructure by phase field simulations. The elongated distorted grains grow and evolve towards equiaxed grains by ideal grain growth. It has been observed that the distortion influences the directional measure of average grain size to a large extent, but the nondirectional average characteristics of the microstructure are not affected.

1. Introduction

Most of the metallic materials are heterogenous at mesoscale and possess a polycrystalline microstructure i.e. an aggregate of grains separated by grain boundaries. Macroscale material properties and functionality depend on its microstructure characteristics including the shape, size, orientation and distribution of the grains. The evolution of microstructure occurs as a result of grain boundary migration. Microstructure evolution is of great technological importance as it can drastically change the material properties in many applications. In recent years, the phase field modeling approach has emerged as a powerful simulation tool for microstructure evolution applications [1–3]. In this approach, the microstructure is represented by a set of non-conserved phase field variables which are continuous in space and time. Each variable represents the local volume fraction of its corresponding phase i.e. it takes unity in its corresponding grain and zero elsewhere. Grain boundaries are modeled as diffuse interfaces across which the phase field variables have a smooth transition. Evolution of the phase field variables under the effect of thermodynamic driving forces implicitly represents grain boundary migration and microstructure evolution.

The most basic form of microstructure evolution is the so-called ideal grain growth that occurs in the *model system* of a polycrystalline aggregate with isotropic grain boundary energy and mobility [4,5]. Such kind of grain growth is driven by the *intrinsic* curvature driving force in order to reduce the total grain boundary energy of a microstructure. On the other hand, there are *extrinsic* driving forces for grain boundary migration such as the heterogeneity in deformation energy of different phases [6–9]. The phase field modeling of ideal grain growth has been extensively investigated during the past years [4,5]. In recent years, phase field models have been extended to include the effect of deformation induced driving forces on grain boundary migration. The modeling efforts of Tonks and Millett [6], Kim et al. [7], Thamburaja and Jamshidian [8], Jamshidian and Rabczuk [9] employ the phase field method to study grain boundary migration in a deformed polycrystalline microstructure. These studies have mainly concentrated on the effect of deformation energy heterogeneity as an *extrinsic* driving force on grain boundary migration. However, they have neglected the

* Corresponding authors. Address: Department of Mechanical Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran (M. Jamshidian). Address: Institute of Structural Mechanics, Bauhaus-University Weimar, Marienstrasse 15, 99423 Weimar, Germany (T. Rabczuk).

E-mail addresses: jamshidian@cc.iut.ac.ir (M. Jamshidian), timon.rabczuk@uni-weimar.de (T. Rabczuk).

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effect of *microstructural distortion* on the kinetics of grain boundary migration by the *intrinsic* curvature driving force. Specifically, these studies neglect the effect of microstructural distortion on the nonlocal gradient energy based on a reasonable assumption for small elastic deformations. However, further development of the phase filed models for finite plastic deformation requires the consideration of such effect. As far as the authors are aware, the only recent work that employs the phase field method to study the ideal growth of distorted grains is the work of Qin [10] basically developed for the simulation of microstructure evolution during steel rolling. Though the first in its kind, this work is limited to the simplest case of a single phase field variable and the simulations are conducted for a system of two adjacent grains. To the best of our knowledge, we have yet to see any *multi-phase* field model which incorporates the effect of microstructural distortion on the kinetics of curvature-driven grain boundary migration.

From a practical point of view, grain topology in polycrystalline metals can be influenced by many factors e.g. compositional and process parameters in solidification [11], heat treatment [12] and deformation processing [13]. Among them, plastic deformation at finite strain can lead to extensive grain distortion. Subsequent to or concurrent with plastic deformation, strain induced grain boundary migration (SIBM) [14,15] and the recently discovered dynamic abnormal grain growth (DAGG) [16–19] phenomena involve the migration of *existing* boundaries and the growth of *existing* grains while prohibiting the nucleation and growth of new grains by recrystallization. In such phenomena while the heterogeneity of deformation energy as an *extrinsic* driving force causes the abnormal growth of a few grains, the concurrent action of the *intrinsic* curvature driving force results in comprehensive evolution of the distorted microstructure. In other words, concurrent with the local intermittent action of the *extrinsic* driving forces, the global permanent action of the curvature driving force constantly contributes to the growth of distorted grains. Crucial is the case of grain growth in deformed nanocrystalline samples where the microstructural length scale is small and inversely the curvature driving force is very high [20–23]. It has been recently shown that for small microstructural length scales, the curvature driving force is the dominant factor for microstructure evolution in stressed grain growth [9]. Therefore, grain growth in deformed nanocrystalline samples can be considered as a related application of ideal growth of distorted grains [24–27].

In this paper, by the term *microstructural distortion* or in short *distortion* we refer to large geometrical deformation of an aggregate of grains. Consequently, a *distorted microstructure* refers to an aggregate of non-equiaxed grains. Following Qin [10], we suppose that such an aggregate is generated by homogenous deformation of an initially equiaxed polycrystalline microstructure. Phase field simulations of ideal grain growth in such a distorted microstructure are performed and the evolution of the distorted grains are investigated. Regardless of how the initially non-equiaxed grains are created, the results obtained from such simulations can be generalized to the evolution of non-equiaxed grains created by processes other than homogenous deformation e.g. solidification [11] or heat treatment [12]. On the other hand, such a *model system* can be extended to include the effect of *extrinsic* driving forces on grain boundary migration for the simulation of microstructure evolution in processes like strain induced grain boundary migration or dynamic abnormal grain growth. Therefore, to allow future extensions and without loss of generality in the present study we assume that the distorted microstructure is created by homogenous deformation of an initially equiaxed grain structure [10].

The plan of the present article is as follows. In Section 2, we develop the phase field theory and derive kinetic relations for the phase field variables. The theory is implemented in a numerical code based on an explicit time integration procedure described in Appendix. The theory and its numerical implementation are then validated by phase field simulations for a benchmark example in Section 3. In Section 4, the developed model is employed to investigate the ideal grain growth in a distorted polycrystalline aggregate by large scale phase field simulations. Finally, in Section 5 the significance and main findings of the present work are discussed and guidelines for future work are given.

2. Phase field theory

Consider a polycrystalline aggregate $\mathcal{B}$ in the *reference* configuration and an arbitrary mesoscale material point identified by the position vector $\mathbf{x} = (x_1, x_2, x_3)$ in $\mathcal{B}$. Each crystal orientation in $\mathcal{B}$ is recognized as a *phase*. The material point $\mathbf{x}$ can be either single-phase representing grain interior or a mixture of multiple phases representing diffuse interface region. Let $\mathbf{y} = \hat{\mathbf{y}}(\mathbf{x}, t)$ denote the position vector of the material point $\mathbf{x}$ in *distorted* configuration and t the real time.

Mathematical Notation: The divergence, gradient and Laplacian operators with respect to the *referential* coordinates $\mathbf{x}$ are denoted by Div, ∇ and ∇^2, respectively. Also, $\nabla\nabla$ denotes the *second* gradient with respect to the *referential* coordinates $\mathbf{x}$. A superimposed dot denotes the material time derivative. Vectors are denoted by bold lower-case Roman alphabets e.g. $\mathbf{a}$ and $\mathbf{b}$; and second-order tensors are denoted by bold upper-case Roman alphabets e.g. $\mathbf{A}$ and $\mathbf{B}$. The zero vector is denoted by $\mathbf{0}$ and the second-order identity tensor is denoted by $\mathbf{I}$. The scalar product between two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{a} \cdot \mathbf{b}$. The dyadic product of the two vectors $\mathbf{a}$ and $\mathbf{b}$ is denoted by $\mathbf{a} \otimes \mathbf{b}$. The transpose of tensor $\mathbf{A}$ is written as $\mathbf{A}^\top$. The inverse of tensor $\mathbf{A}$ is written as $\mathbf{A}^{-1}$. The determinant of tensor $\mathbf{A}$ is denoted by $\det \mathbf{A}$. The product between two tensors $\mathbf{A}$ and $\mathbf{B}$ is denoted by $\mathbf{AB}$. The scalar product between two tensors $\mathbf{A}$ and $\mathbf{B}$ is denoted by $\mathbf{A} : \mathbf{B}$.

The distortion of $\mathcal{B}$ is characterized by the *mesoscale* deformation gradient $\mathbf{F} = \nabla\mathbf{y}$. Following Kalidindi et al. [28], Thamburaja and Jamshidian [8] and Jamshidian and Rabczuk [9] we employ the Taylor homogenization method and assume that the distortion is homogenous throughout $\mathcal{B}$. As a reasonable assumption for finite deformation of metallic materials, we also assume that the distortion is *isochoric* i.e. volume conserving. We further assume that the polycrystalline aggregate is distorted through a distortion-controlled process. In rigorous mathematical form,

$$\mathbf{F}(\mathbf{x}, t) = \hat{\mathbf{F}}(t) \quad \text{for} \quad \mathbf{x} \in \mathcal{B} \quad \text{with} \quad \det \hat{\mathbf{F}}(t) = 1, \tag{1}$$

where $\hat{\mathbf{F}}(t)$ is a *prescribed* deformation gradient for all time t. The volume fraction of phase i in the mesoscale material point $\mathbf{x}$ in the *reference* configuration is denoted by the *referential* phase field variable $\phi_i = \hat{\phi}_i(\mathbf{x}, t)$ with $i = 1, 2, \ldots, N$, where N is the total number of different phases/crystal orientations in $\mathcal{B}$. As the volume fraction, ϕ_i has physical bounds of $0 \leqslant \phi_i \leqslant 1$ and is constrained by the physical constraint $\sum_{i=1}^{N} \phi_i = 1$. The phase field theory is developed for a typical mesoscale material point in the *reference* configuration. Particularly, the local free energy functional and consequently the phase field kinetic relations are expressed and derived in terms of *referentially* defined variables.

As a measure of distortion, let $\mathbf{C} = \mathbf{F}^\top\mathbf{F}$ denote the *mesoscale* right Cauchy–Green deformation tensor defined over $\mathcal{B}$ at all time t. Along with the principle of material frame-indifference which ensures that the free energy and phase field kinetic relations are independent of the referential frame, we assume the following functional form for the local free energy per unit *reference* volume as

$$\psi = \hat{\psi}(\mathbf{C}, \phi_1, \ldots, \phi_N, \nabla\phi_1, \ldots, \nabla\phi_N), \tag{2}$$