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Phase-field modeling of displacive phase transformations in elastically anisotropic and inhomogeneous polycrystals

Tae Wook Heo [a,*], Long-Qing Chen [b]

[a] Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
[b] Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA

Abstract

We integrate the inhomogeneous elasticity model and the phase-field equations for displacive phase transformations in polycrystalline materials. The relaxation of the misfit strain between parent and transformed product phases or among different structural variants of transformed product phases near grain boundaries is taken into account. It is applied to the *fcc* to *bcc* martensitic transformation described by a Bain strain in a polycrystalline Fe-31at.%Ni metallic alloy. The focus is on the effect of grain boundaries on the displacive transformation behaviors. We first study nucleation of the *bcc* product phase at a grain boundary of a bicrystal. The predicted microstructures through nucleation near grain boundaries are compared to existing experimental observations in literature. The effects of grain boundary characteristics such as the degree and range of the misfit strain relaxation at the grain boundary and grain boundary curvature on the phase behaviors near a grain boundary are then examined for both a flat or a curved grain boundary. The model is also applied to polycrystals containing multiple grains. The effects of the misfit strain relaxation at grain boundaries, elastic anisotropy, and applied stress on the kinetics and the microstructures of displacive transformations are discussed.

Keywords: Displacive phase transformation; Inhomogeneous elasticity; Elastic anisotropy; Polycrystals; Phase-field model

1. Introduction

Displacive phase transformations are common in a wide spectrum of materials ranging from metals to ceramics when a system is subject to temperature variation and/or mechanical deformation [1–6]. In many cases, a displacive transformation involves a change in crystal symmetry. Examples include the *bcc* to *hcp* transformation in titanium alloys [7], the *fcc* to *bcc* Bain transformation in steels [3], and the *hcp* to *fcc* structural change during hydride formation in zirconium alloys [8], to name just a few. A displacive transformation is accomplished by an atomic or crystal lattice rearrangement, i.e., atomic shuffle and/or lattice distortion [1], driven by the chemical free energy reduction, resulting in multiple crystallographically equivalent structural variants of the product phase. The accommodation of lattice misfit between the structural variant and the parent phase or among domains of different orientations generates a significant amount of strain energy, and the relaxation of strain energy leads to complex self-assembling domain microstructures.

Structural defects such as dislocations, grain boundaries, precipitates or inclusions, free surfaces, etc. often play significant roles in the displacive transformation behavior by modifying the nucleation or kinetic barriers. In particular, grain boundaries in polycrystals can act as heterogeneous nucleation sites. Although there have been efforts to elucidate the effects of grain boundaries [9–11], it is still extremely challenging to experimentally capture

* Corresponding author.
E-mail addresses: heo1@llnl.gov, htw584@gmail.com (T.W. Heo).

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the phase transformation kinetics and microstructural features during displacive structural changes since the transformations are very rapid and they produce complex microstructures. In addition, the presence of structural defects adds complexity to the transformation behaviors. Hence, there have been a number of theoretical and/or computational efforts [12–19] to uncover the underlying mechanisms and physics of displacive phase transformations. Phase-field method [20–25] based on the diffuse-interface description [26] has been successfully developed and employed to tackle the problems related to the displacive transformations [2]. The first successful three-dimensional phase-field model for the martensitic transformation, one type of displacive phase transformations [1], was proposed by Wang and Khachaturyan [27]. The model was developed for modeling the improper martensitic transformation and successfully employed to produce microstructural features during the nucleation, growth, and coarsening of the martensitic phase in the parent phase of a single crystalline metallic alloy. A phase-field model for a proper martensitic transformation was also proposed [28]. A similar modeling framework has been adopted for modeling several types of crystal symmetry changes with or without diffusional processes [29–36]. Recently, the elasto-plastic effects have been incorporated to phase-field modeling of martensitic transformations by incorporating the dislocation dynamics [37,38], and the elasto-plastic phase-field model [39] was applied to simulating the martensitic transformations by introducing a local plastic yielding criterion [40–45]. In addition, a vector model based on the phase-field theory for the proper displacive phase transformations has also been proposed to take into consideration the structural anisotropy and directional flexibility [46]. The phase-field models for martensitic transformations have been extended to study the transformation behaviors near structural defects such as dislocations [47], precipitates [48], free surfaces [49], void, stress-concentration sites, and inert inclusions [50], and to study the transformation behaviors in a thin film constrained by a substrate [51,52] or in a multilayer system consisting of alternating active and inert layers [53]. General reviews of phase-field models for the martensitic transformation are available in Refs. [54,55]. They have been also extended to model microstructure evolution during martensitic transformations in polycrystals [45,56–60]. These models captured the essential features of the phase behavior in the presence of multiple grains. However, some details of the microscopic features near grain boundaries, e.g., heterogeneous nucleation of variants near grain boundaries, were not analyzed. In existing phase-field simulations, pre-existing nuclei inside a grain were employed in most of the simulations in the absence of external loading, or external loading was applied to trigger the transformation inside grains or near grain boundaries [59]. In addition, all existing models are based on the isotropic homogeneous elasticity approximation although the models take into account the rotation of the transformation strain associated with the crystallographic orientation variation from one grain to another. Finally, existing models also ignore the possible misfit strain relaxation or loss near a grain boundary.

In this paper, we describe phase-field kinetic equations for modeling displacive phase transformations in elastically inhomogeneous and anisotropic polycrystals [61,62]. In particular, the possible misfit strain relaxation or coherency loss at the grain boundaries is incorporated to capture the microscopic phase behaviors near the grain boundaries. The martensitic transformation in Fe-31at.%Ni alloy is employed as an example to study the generic features of the displacive transformation [1]. It will be the basis for our phase-field modeling of the phase transformations and coupled microstructure evolution in polycrystalline alloys where both diffusional and displacive transformations take place.

2. Phase-field modeling

During a displacive structural transformation, multiple variants of the product phase are produced. The number of possible variants is determined by the symmetry of the crystal lattice rearrangement [17,27]. For example, the *fcc* to *bcc* Bain transformation produces three crystallographically equivalent variants due to the tetragonal symmetry of the transformation strain, i.e., the tetragonal axis of the strain can be aligned with any one of the three crystallographic directions [1 0 0], [0 1 0], and [0 0 1] in a cubic lattice. Therefore, multiple structural order parameters are required accordingly in order to account for the structural change within the phase-field context. In addition, for polycrystals, each grain contains its own set of structural order parameters [57]. Hence, we define the structural order parameter (or phase-field) $\eta_{pg}(\vec{r},t)$ where p represents the structural variant index and g represents the grain index in order to identify multiple structural variants in each grain. For instance, $p = 1, 2, 3$ and $g = 1, 2, \ldots, N$ for the *fcc* to *bcc* Bain transformations in a polycrystal containing N grains. Recently, Malik et al. employed continuous structural order parameters across a grain boundary and they regarded a grain boundary as a kinetically frozen phase, acting as a kinetic barrier at the grain boundary, by varying the kinetic coefficient of the governing equation to account for the discontinuity of the transformation process across the grain boundary [59,60]. It should be noted that our definition automatically takes into account the discontinuity of the structural order parameter across the grain boundary without specific considerations at the grain boundary and without the significant loss of computational efficiency (see Section 2.3 and Supplementary Material S1). The total free energy functional of the entire system is expressed as the following volume integral [27,57]:

$$F = \int_V \left\{ f(\{\eta_{pg}\}) + \sum_g \sum_i \sum_j \sum_p \frac{\kappa_{p,ij,g}}{2} \nabla_i \eta_{pg} \nabla_j \eta_{pg} + e_{\text{coh}} \right\} d^3\vec{r}, \qquad (1)$$