Commun. Comput. Phys.
doi: 10.4208/cicp.290610.060411a

Vol. **11**, No. 3, pp. 726-738
March 2012

A Spectral Iterative Method for the Computation of Effective Properties of Elastically Inhomogeneous Polycrystals

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Received 29 June 2010; Accepted (in revised version) 6 April 2011

Available online 28 October 2011

Abstract. We report an efficient phase field formalism to compute the stress distribution in polycrystalline materials with arbitrary elastic inhomogeneity and anisotropy. The dependence of elastic stiffness tensor on grain orientation is taken into account, and the elastic equilibrium equation is solved using a spectral iterative perturbation method. We discuss its applications to computing residual stress distribution in systems containing arbitrarily shaped cavities and cracks (with zero elastic modulus) and to determining the effective elastic properties of polycrystals and multilayered composites.

AMS subject classifications: 74B10, 74S25

Key words: Elasticity, spectral method, iterative method.

1 Introduction

Phase-field models have been extensively used to study the effect of elastic stresses on microstructural evolution during solid-to-solid phase transformations (see the reviews [1–3] for details). However, most of these models approximate the elastic modulus to be homogeneous. Homogeneous modulus approximation is not a valid assumption when the microstructures exhibit large elastic inhomogeneity. Examples of elastically inhomogeneous materials include multiphase materials in which the constituent phases have different elastic moduli, composites, systems containing cavities and cracks, and polycrystalline materials. In the case of polycrystals, the overall elastic stiffness tensor depends

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on the orientation of each grain constituting the polycrystal. As a result, polycrystalline materials are always associated with an inhomogeneous distribution of elastic moduli.

There have been fewer efforts to model elastically inhomogeneous systems using phase field models. Leo et al. and Zhu et al. numerically solved the mechanical equilibrium equation for elastically inhomogeneous systems using conjugate gradient method [4, 5]. Hu and Chen developed an iterative-perturbation scheme to solve the mechanical equilibrium equation in elastically inhomogeneous binary alloys [6, 7]. Wang et al. developed a phase field microelasticity theory to model elastically and structurally inhomogeneous solids [8]. Their theory is based on the estimation of strain energy of an elastically inhomogeneous solid by numerically computing the effective stress free strain for an equivalent elastically homogeneous system [8, 9].

In this paper we present a phase field model based on the iterative-perturbation method developed by Hu and Chen [6] to compute the residual stress distribution in polycrystalline materials. This allows one to compute the equilibrium stress distribution for any arbitrary structurally and elastically inhomogeneous microstructure using our method. Furthermore, it will be shown that the effective elastic properties of polycrystals can be efficiently computed from its response to an applied stress or strain.

2 Formulation and numerical implementation

In the phase-field model developed by Fan and Chen for studying grain growth [10, 11], a polycrystalline microstructure is described using a set of Q continuous, non-conserved order parameter fields $\eta_i(\mathbf{r},t)$ $(i=1,\cdots,Q)$. The order parameter fields represent grains of a given crystallographic orientation. We use a function $\phi(\mathbf{r},t)=\sum_i \eta_i^2(\mathbf{r},t)$ to distinguish between the grain interior and the grain boundaries.

In a polycrystalline material, the elastic constants depend on the relative orientation of different grains constituting the polycrystal and hence are always inhomogeneous. Since the grains are rotated with respect to a fixed coordinate system, the elastic stiffness tensor for each grain is obtained by transforming the tensor with respect to the fixed coordinate system. Let C_{ijkl} represent the stiffness tensor for a single grain in a fixed reference frame. Then, the position-dependent elastic stiffness tensor for the entire polycrystal in terms of the order parameter fields is defined as

$$C_{ijkl}(\mathbf{r})=\sum_g \eta_g^2(\mathbf{r}) a_{ip}^g a_{jq}^g a_{kr}^g a_{ls}^g C_{pqrs}, \tag{2.1}$$

where a_{ij}^g is the transformation matrix representing the rotation of the coordinate system defined on a given grain 'g' with respect to the fixed reference frame and C_{pqrs} is the stiffness tensor of the reference medium. The transformation matrix a_{ij} is expressed in