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Two-step homogenization simulation for multidomain and multigrain structures in piezoelectric materials

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Abstract

In this paper, a two-step scale-up procedure based on asymptotic homogenization theory is proposed for hierarchical structures consisting of multigrains and multidomains in piezoelectric materials. Intragranular domains are modeled as a microstructure during the first-step homogenization. Then, in the second-step homogenization, an aggregate of randomly oriented grains is modeled by applying the first-step homogenized material properties of multidomains to every grain. A dual-domain structure consisting of positive and negative directional domains with a 180° orientation gap is computed for case study analysis. The three-dimensional electron backscatter diffraction-measured microstructure is employed for the multigrain structure. The effect of the domain configuration on the macroscopic homogenized material properties of polycrystalline piezoelectric materials is investigated through the two-step homogenization process. In particular, the material property changes caused by the piezoelectric effect, which cannot be estimated by the mixture law, are discussed for multigrain and multidomain structures.

Keywords: Piezoelectric material; Multiscale analysis; Homogenization modeling; Multidomain; Multigrain

1. Introduction

Ferroelectric materials, of which the best known is lead zirconate titanate (PZT), are widely used for various electromechanical devices because they exhibit excellent piezoelectric performance. In particular, many PZT-actuated and PZT-sensing microelectromechanical systems [1–4] have been developed using advanced micro- and nanotechnology. These have found application in a wide range of fields, from information and automobile devices to chemical, healthcare and medical equipment.

The important characteristics of ferroelectric materials stem from their noncentrosymmetry, typified by the tetragonal and rhombohedral perovskite-type crystal structures. These noncentrosymmetric crystal structures have a spontaneous polarization whose direction switches to the opposite or transverse direction under an external load. This phenomenon, called domain switching, is the most interesting feature of ferroelectric materials. Domain switching creates a complicated multidomain structure in every grain and has a significant influence on the effective material properties.

Many computational approaches, such as nonlinear material modeling [5–11], thermodynamic modeling [12–14] and phase-field modeling [15–18], have been developed to explain the domain switching behavior in ferroelectric materials. If one focuses on modeling of the domain configuration, computational approaches can be classified into two types: (i) single-domain models [5–7], where, for simplicity, every grain in a polycrystalline material is assumed to be uniform, with no domain walls present; and (ii) multidomain models, further subdivided into direct [12–18] and indirect modeling approaches [8–11]. The former approach

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models an inhomogeneous domain structure directly when the microstructural region is discretized. Although direct modeling restricts the analytical region of the microstructure to a small number of grains or two dimensions because of the huge computational cost, it reveals details of domain switching behavior. However, it is generally difficult to determine global material properties because of the limited microstructure, which is not large enough to be a representative volume element. The latter approach indirectly takes into account the effect of the multidomain structure by employing the mixture law or inclusion theory. These models allow overall material properties and behaviors to be determined, since simple modeling of multidomain structures enables utilization of a large microstructure model, which can serve as a representative volume element. The mixture law calculates every component of the effective material properties through the summation of products of the corresponding component with the volume fraction. The mixture law is useful for simple inhomogeneous structures in cases where the material properties are independent of each other. However, the elastic and dielectric constants of piezoelectric materials cannot be determined independently because of the coupling effect. It is necessary to consider not only the volume fraction, but also the interaction of material properties. However, asymptotic homogenization theory [19] enables analysis of arbitrary configurations of microstructure and consideration of the interaction of material properties. In a previous study, a multiscale finite element simulation based on the homogenization theory was developed for the problem of coupling between mechanical displacement and electric potential [20,21]. Crystal morphologies of polycrystalline piezoelectric materials were modeled into a microstructure, and then macroscopic homogenized properties of polycrystalline piezoelectric materials were estimated by employing the three-dimensional (3-D) electron backscatter diffraction (EBSD)-measured microstructure [22]. Meanwhile crystal orientations of a microstructure were optimized, and the macroscopic piezoelectricity of a polycrystal was upgraded successfully beyond that of a single crystal [23]. However, these computations assumed that every grain contained a single domain. They did not take into account any multidomain configurations. Both multigrain and multidomain structures require that scale-bridging be applied on the basis of mathematically rigorous formulations. It remains an important challenge to apply homogenization theory to the hierarchical modeling of multigrain and multidomain structures in piezoelectric materials.

In this paper, a two-step homogenization procedure based on asymptotic homogenization theory is proposed for hierarchical structures consisting of multigrains and multidomains in piezoelectric materials. The first and second steps of the homogenization are for intragranular domains and randomly oriented grains, respectively. A dual-domain structure, i.e., 0° and 180° domains, was computed for case study analysis. In addition, the 3-D EBSD-measured microstructure [22] was employed for the multigrain structure. The focus is on the linear piezoelectricity problem, and the effect of domain configuration on macroscopic homogenized material properties of polycrystalline piezoelectric materials is investigated through a two-step homogenization process. In particular, material property changes caused by the piezoelectric effect, which cannot be estimated by the mixture law, were discussed for multigrain and multidomain structures.

2. Numerical modeling of hierarchical structures

Piezoelectric materials generally have a hierarchical structure consisting of many grains and domains at the microscopic scale. Fig. 1 illustrates the crystal morphology of real piezoelectric materials. Fig. 1a shows the atomic force microscopy (AFM) image of unpoled polycrystalline barium titanate ($BaTiO_3$). The specimen surface was corroded with sulfuric acid. The surface undulation reveals the aggregation of many grains and voids. In particular, owing to the difference in corrosion effect between the positive and negative surfaces of spontaneous polarization in a domain, a typically streaky microstructure, the 0°/180° domain structures in the grains, is observed. Fig. 1b shows the EBSD-measured crystal orientations for unpoled polycrystalline PZT. It indicates that many grains with different crystal orientations form a complicated texture. Focusing on extended EBSD images for some grains, one can see that the 0° and 90° domain structure can be detected from the difference in lattice constant between the vertical and transverse directions of spontaneous polarization. For these ferroelectric materials, such as $BaTiO_3$ and PZT, the direction of spontaneous polarization switches to the opposite or transverse directions under external load. Domain switching creates an inhomogeneous domain structure in grains and changes the piezoelectric properties drastically. Thus, a two-step homogenization simulation to determine material properties is proposed, taking into consideration multigrain and multidomain structures. Fig. 2 shows the overall scheme of the proposed two-step homogenization simulation for polycrystalline piezoelectric materials. The first step is the homogenization of intragranular multidomain structures, which are 0°/180° and 0°/90° domain structures in the case of tetragonal crystals. This first step determines the effective material properties for every grain. The second step involves the homogenization of an aggregate of multi-oriented grains to estimate the macroscopic material properties.

In this study, the asymptotic homogenization theory, which can bridge two different scale-coupling problems between the macrostructure and the microstructures, was employed for the first- and second-step homogenization. As details of the formulations and computational techniques based on asymptotic homogenization theory for the piezoelectric coupling problem have been reported elsewhere [20–23], the essence of the homogenization process is described briefly in this section. Fig. 3 illustrates the scheme of the homogenization modeling. Macrostructures are