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Anisotropic phase field solution for morphological evolution and migration of inclusions in piezoelectric films

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ABSTRACT

Based on an anisotropic phase field model, the morphological evolution and migration of inclusions in piezoelectric films under mechanical and electric loads are investigated. An order parameter field is introduced to characterize the evolution of inclusion in piezoelectric film, where the zero contour evolution of order parameter in the phase interface layer between inclusion and matrix film tracks the morphological change and migration of the inclusion driven by coupled mechanical and electric loads. Results show that morphological evolution and migration of inclusion in piezoelectric film is mainly caused by normal stress gradient in the phase interface layer between inclusions and piezoelectric film, and when piezoelectric film appears in a lower resistivity, an additional drive force induced by electron field (electron wind) exerted the piezoelectric film promotes the migration of an inclusion toward the higher electric potential direction. Anisotropic diffusion behavior of interface layer causes asymmetrically morphological evolution of inclusion in piezoelectric film under different loads.

1. Introduction

Due to coupled electromechanical behaviors, piezoelectric materials have been widely used as electronic instruments, sensor and artificial intelligence elements [1–6]. In processing piezoelectric elements, various damage defects, such as inclusions and voids, are often generated, which makes the coupled electromechanical characteristics of piezoelectric materials be affected in engineering applications. It is seen from the theoretical analysis and experimental observation that the evolution, migration and coalesce of void (inclusion) defects in PZT (Lead zirconate titanate) materials may cause the damage of some smart devices and reduce their life span [7]. The contamination of inclusions affects the reliability of electronic elements [8–13]. All these situations have detrimental effects on the function of film structures [14,15]. Thus, it has become a big challenge for microelectronic industries. A good investigation into the effect of defect on the function of piezoelectric materials is needed.

Many investigations on coupled electromechanical characteristics of piezoelectric materials with inclusion were presented in Refs. [16–24]. By means of an analytical method, Wang and Zhong investigated the problem of a conducting arc crack between a circular piezoelectric inclusion and an infinite piezoelectric matrix [16]. Shen et al. [17] reported an investigation into the interaction of a piezoelectric screw dislocation with a nonuniformly coated circular inclusion in piezoelectric film

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Nomenclature

ϕ	order parameter
$C_{ij}(\phi)$	the elastic coefficients of phase interface layer
$q_{ij}(\phi)$	the piezoelectric parameters of phase interface layer
$\eta_{ij}(\phi)$	the permittivity constants of phase interface layer
C_{ij}^{M}, q_{kl}^{M}, η_{mn}^{M}	the material properties of piezoelectric film
C_{ij}^{I}, q_{kl}^{I}, η_{mn}^{I}	the material properties of inclusion
λ	defect parameter
σ_{ij} and ε_{ij}	stress components and strain components
E_l and S_l	electric field strength and electric displacement
W_P and W_E	strain energy density and electric potential energy density
γ_i	interfacial energy per unit area
β	the volume of phase interface layer
Ω	atom volume
κ	interface curvature
δ_i	the thickness of interface layer
J	atomic flux density
k	Boltz-mann's constant
T	absolute temperature
D_i	isotropic lattice diffusion coefficient
Q_s	the activation energy for interface diffusion
σ_n	the normal stress of interface layer
g_d	anisotropic coefficient
η_0	the vacuum permittivity of piezoelectric

subjected to remote antiplane shear and electric fields. Based on complex variable method, Yang and Gao investigated the plane problems of multiple piezoelectric inclusions in a non-piezoelectric film [18]. Wang and Zhou investigated the internal electroelastic field within a three-phase piezoelectric inclusion with arbitrary shape when the piezoelectric film is subjected to remote uniform electroelastic loadings [19]. By utilizing the Euler–Bernoulli beam model and Rayleigh–Rita approximation technique, Della and Shu gave a mathematical model for vibration of beams with piezoelectric inclusions [20]. Kuvshinov [21] presented explicit and closed-form solution for electroelastic deformations due to polyhedral inclusion in uniform half-space and bi-materials utilizing Green function method. Fakri and Azrar [22] predicted the electroelastic and thermal responses of piezoelectric composites with and without voids. By extending the double inclusion model to multiphase with piezoelectric layers, Lin and Sodano [23] investigated the electroelastic properties of the multifunctional composites. Aldraihem [24] developed a comprehensive micromechanics model to estimate the effective viscoelastic properties of hybrid composites containing polymer matrix.

In above investigations into the influence of inclusions in matrix on the mechanical and electric characteristics of smart structures, the inclusions are fixed at a determinate point in matrix. In fact, under thermal mismatching and electric field, the inclusions in matrix may migrate to a new point in the matrix. Qin et al. [25] presented an analytical method to solve the migration velocity of inclusion in piezoelectric film under coupled gradient stress and electric field, in which the inclusion keeps its original shape and moves at a constant speed.

In general, the shape and migration velocity of inclusion in solid is variable in migrating process. Therefore, the investigation on the morphological evolution and migration move of inclusion in solid is more close to practical problem. Using phased field model, Li et al. [26] investigated the electromigration-driven morphological evolution and migration of inclusion in finite scale interconnects, in which morphological evolution and migration of an inclusion in finite scale interconnects are proportional to the electric field strength exerted on the interconnects. Bhate et al. [27] presented the current-driven interaction between voids in metallic interconnects, in which surface diffusion is the main mechanism for the electromigration of void. However, due to the coupled electroelastic behaviors of piezoelectric solid with defects is complex, the investigation into the morphological evolution and migration of inclusions in finite scalar piezoelectric film is not presented in literatures so far.

In this paper, the phase field model for the interface evolution between inclusion and piezoelectric film is found to simulate the morphological evolution and migration of inclusion in finite scalar piezoelectric film with high resistivity or low resistivity, under different loads. Here, the interface diffusion behavior between inclusion and piezoelectric film may be anisotropic, the initial shape of inclusions is arbitrary, and the external loads exerted on piezoelectric film are considered as uniformly distributed load, gradient load and electric load. Results show that the morphological evolution of inclusion mainly occurs in the regions with the larger normal stresses along the arc length of phase interface layer, and the morphological evolution of inclusion in piezoelectric film with higher resistivity is mainly induced by exerted mechanical loading. The tip of wedge-shaped inclusion defects in piezoelectric film under gradient stress in *y*-direction appears in a degradation