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Migration velocity of an elliptical inclusion in piezoelectric film

Y. Qin, X. Wang *

School of Naval Architecture, Ocean and Civil Engineering (State Key Laboratory of Ocean Engineering), Shanghai Jiaotong University, Shanghai 200240, PR China

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ABSTRACT

This paper presents an analytical method to investigate on the migration velocity of an elliptical inclusion in piezoelectric film under coupled gradient stress and electric field. The effects of gradient stress, electric field, the material property and the shape parameter of inclusion on the migration velocity of the elliptical inclusion in piezoelectric material are described and discussed.

1. Introduction

In the past, many investigations on the use of piezoelectric materials have already been presented for active control of smart structures with light weight. The inherent electromechanical effect of piezoelectric materials has many important engineering applications [1–6]. Current examples motivating the present study are strained semiconductor laser devices [7,8], in which residual stresses induced by lattice mismatch between buried active components and surrounding materials crucially affect electronic performance. In processing of thin films, various structural defects such as inclusions and voids in the thin film are often generated, which have detrimental effects on the function of film structures [9,10]. Investigations on mechanical deformations induced by misfitting inclusions in an infinite or semi-infinite piezoelectric medium are fundamental physical and engineering problems, which can be seen in earlier researches on this subject by Nowacki [11] and Mura [12].

Because of the rapid development of piezoelectric smart structures in the last years, many related works on coupled electromechanical characteristics of piezoelectric material with inclusions are further investigated by many researchers [13–17]. Della and Shu [13] utilized the Euler–Bernoulli beam theory and Rayleigh–Ritz approximation technique to present a mathematical model for the vibration of beams with piezoelectric inclusions. Based on the linear elasticity theory and Green's function method, Kuvshinov [14] presented explicit, closed-form expressions to describe electroelastic deformations due to polyhedral inclusions in uniform half-space and bi-materials. Fakri and Azrar [15] predicted the electroelastic and thermal responses of piezoelectric composites with and without voids. Lin and Sodano [16] extended the double inclusion model to multiphase composites with piezoelectric layers, and predicted the electroelastic properties of the multifunctional composites. Based on the viscoelastic principle, Aldraihem [17] developed a comprehensive micromechanics model to estimate the effective viscoelastic properties of hybrid composites containing polymer matrix. Tang et al. [18] reported that the energy density of the nanocomposite could be significantly increased through the use of piezoelectric nanowires and a polymer with greater breakdown strength. It is seen from Ref. [19] that strain-release characteristics of composites are reinforced by nanowires on stretchable substrates. Utilizing dielectrophoretic assembly, Tomer and Randall [20] make anisotropic composites reinforced by BaTiO3 particles in a silicone elastomer thermoset polymer, and investigate the effect of electrical properties on the property of these composites. It is described in Ref. [21] that the energy-storage capability of the nanocomposite can be enhanced by the alignment of piezoelectric nanowires in the direction of the applied electric field compared to randomly oriented samples.

In the above investigation into the influence of inclusions in piezoelectric materials on the mechanical and electrical characteristics of piezoelectric smart structures, the inclusion is fixed at a determinate point in piezoelectric material. In fact, the various solid films with inclusion are often subjected to severe gradient stresses induced by thermal mismatching and electric field, so that the inclusion in films may migrate [22–25]. Because one of the major damage mechanisms is from the inclusion (void) coalescence in stress concentration region induced by the motion of inclusion (void), the dynamics of stress-driven inclusion in metallic solids has been generating great research interest for the failure of metallic interconnects in integrated circuits [26–28]. Utilizing self-consistent numerical method, Gungor and Maroudas [30] describe the effects of complex external stresses on the electromigration-driven motion of morphologically stable voids in elastically deforming metallic thin films, and reveal the complex evolution of voids. It is seen in

* Corresponding author.
E-mail address: xwang@sjtu.edu.cn (X. Wang).

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Ref. [31] that when the morphological stability limit is approached, the void migration speed is substantially dependent on the void size. Therefore, the inclusion migration-induced failure should also pose a great concern in piezoelectric smart structures. However, because the coupled electroelastic characteristic of piezoelectric material with inclusion is complex, the investigation on the migration of inclusion in piezoelectric film is not found in literatures so far.

In this paper, we give an analytical solution for the migration of an elliptical inclusion in piezoelectric film under coupled gradient stress and electric field, based on the atomic migration principle in a diffused interface layer between inclusion and piezoelectric matrix from regions of high chemical potential to those of low chemical potential along the interface layer. The numerical examples describe the effects of gradient stress, electric field, and the material property and the shape of inclusion on the migration velocity of the elliptical inclusion in piezoelectric film. The present work may stimulate further interest on this topic because the reliability of piezoelectric smart structures is extremely sensitive to inclusion defects.

2. Basic equations and solving method

Fig. 1 shows the two-dimensional (2D) model of an elliptic inclusion in piezoelectric film under coupled gradient stress and electric field, in which this 2D implementation conveys the essence of a three-dimensional (3D) problem of inclusion in piezoelectric material, and represents an inhomogeneity extending throughout the thickness along z, consistently with experimental observations in thin-piezoelectric film. In order to obtain the strict stress and electric field solutions at the interface required in the present derivation, the calculating model in Fig. 1 is based on the migration of inclusion in an infinite piezoelectric material under the combined electric and stress gradient loads, in which its realistic application in a finite-width piezoelectric film will exist in scale effects. However, Li and Chudnovsky [32] have proved that the scale effect is negligible when the ratio of inclusion size to a characteristic size of the analytical system is less than 0.15 by using the method of numerical analyses. Because the characteristic size of the analytical system for an inclusion in a finite piezoelectric film is the width of the film, the present model can be used to calculate the inclusion motion in a realistic piezoelectric film when the inclusion size is much less than the width of film.

At infinity, the model is subjected to gradient stress field $q_y = pX$ in the Y direction by thermal mismatch, where $p = {}^{dq_y}\!/_{dX}$ is a constant, a positive value of p presents a rising stress along the X-axis, while in the X-direction subjected to electric field E_0. In Fig. 1, the global coordinate system OXY is fixed at the symmetric center of piezoelectric film, the local (moving) coordinate system oxy is fixed at the center of an elliptic inclusion, and x_L represents a moving distance from the center of the elliptic inclusion to the symmetric center of piezoelectric film. The relation between the two coordinate systems is given by $x_L = X - x$ and $y = Y$.

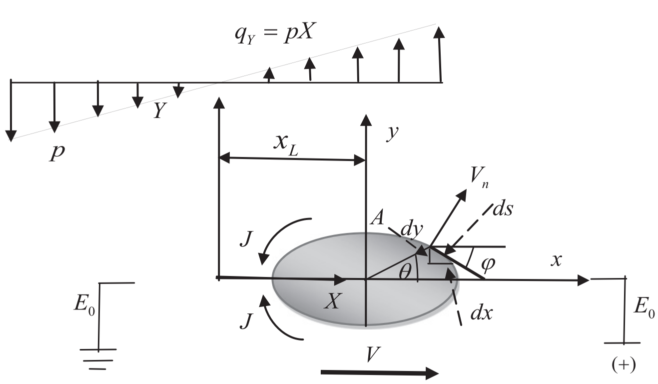

Fig. 1. The motion of an elliptical inclusion in infinite piezoelectric material under combined gradient stress field and electric field.

The constitutive relations of orthotropic piezoelectric film are written as [29]

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = \begin{bmatrix} S_{11} & S_{13} & 0 \\ S_{13} & S_{33} & 0 \\ 0 & 0 & S_{44} \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} + \begin{bmatrix} 0 & d_{31} \\ 0 & d_{33} \\ d_{15} & 0 \end{bmatrix} \begin{Bmatrix} E_x \\ E_y \end{Bmatrix} \tag{1a}$$

$$\begin{Bmatrix} D_x \\ D_y \end{Bmatrix} = \begin{bmatrix} 0 & 0 & d_{15} \\ d_{31} & d_{33} & 0 \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} + \begin{bmatrix} e_{11} & 0 \\ 0 & e_{33} \end{bmatrix} \begin{Bmatrix} E_x \\ E_y \end{Bmatrix} \tag{1b}$$

where $\sigma_x, \sigma_y, \tau_{xy}$ and $\varepsilon_x, \varepsilon_y, \gamma_{xy}$ are, respectively, stresses and strains in the piezoelectric film along the main direction of coordinate system oxy, E_x, E_y and D_x, D_y are, respectively, the electric field strengths and the electric displacements along the x and y directions, S_{ij} is the flexible coefficients of piezoelectric film, and d_{ij} and e_{ij} are the piezoelectric and dielectric constants, respectively.

The inclusion in piezoelectric film may be moved by the atomic migration of an inclusion/matrix interface layer from bulk regions of high chemical potential to those of low chemical potential along the interface layer. Because the interface diffusion is generally much faster than the bulk one, only the interface diffusion is considered as the major mechanism for the inclusion motion in piezoelectric film under coupled gradient stress and electric field. In general, instable inclusions including very narrow morphologies may be split into small inclusions with stable shape to minimize the total Gibbs free energy of the system under external loads. In order to give an analytical solution for the migration velocity of an inclusion in piezoelectric film under coupled field, it is assumed in this analytical model that the inclusion is considered as an elliptic inclusion with shape parameter m, and the morphology of the elliptic inclusion is taken to be stable throughout the range of the shape parameters when the inclusion simply migrates along the length direction of film.

Because the shape and size of an inclusion in piezoelectric film do not change during motion, the piezoelectric film is the source and sink for the atomic flux along the interface layer between inclusion and piezoelectric matrix. Under coupled gradient stress and electric field, atoms diffuse along the interface layer from one side of high chemical potential to the other of lower, so that the inclusion migrates in the piezoelectric matrix against the migration of the atoms. Thus, the chemical potential in the interface layer driving this atomic flux is composed of the free energy, the local elastic strain energy and the local electric energy in the interface layer, as follows

$$\mu = \mu_0 - \Omega\gamma_i\kappa - \Omega\sigma_n + \Omega W_p + \Omega W_E, \tag{2}$$

where μ_0 is the reference value of the potential, γ_i is the free energy of interface layer, κ is the surface curvature of the inclusion, positive for convex, Ω is the atomic volume, σ_n is the normal stress on the inclusion surface, W_p is the elastic strain energy density stored in the interface layer associated with an atom, as follows

$$W_p = \frac{1}{2}(\sigma_n\varepsilon_n + \sigma_\theta\varepsilon_\theta + \tau_{n\theta}\gamma_{n\theta}), \tag{3a}$$

and W_E is the electric energy density stored in the interface layer associated with an atom, as follows

$$W_E = \frac{1}{2}(E_nD_n + E_\theta D_\theta) \tag{3b}$$

where D_n, D_θ and E_n, E_θ represent, respectively, electric displacements and electric strength along the normal n and circumference θ of the interface layer.