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Effects of material mismatch on interfacial cracking of ferroelectric film/substrate structures

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A B S T R A C T

This study investigates the effect of material mismatch on interfacial cracking in ferroelectric film/substrate structures, models the interfacial misfit strain using a Somigliana screw dislocation dipole, and solves the generalized stress functions, the stress intensity factor (SIF) and the electric displacement intensity factor (EDIF) in piezoelectric coupled field based on an equivalent model and the complex potential method. The results show that: (1) The lattice mismatch degree is the major factor influencing EDIF and SIF; (2) The effects of the elastic and dielectric constant ratios of substrate to film on EDIF depend on the mismatch effects resulting from the other two constant ratios of generalized stiffness, respectively, however the piezoelectric constant ratio can affect EDIF independently; (3) The increasing elastic constant ratio can lead to a monotonic and significant increase of SIF; and when the piezoelectric constant ratio is greater than 1, it can cause an obviously change in SIF; however dielectric constant ratio has little effect on SIF; and (4) The modest adjustment of the piezoelectric constant ratio within a specific range could be a potential route to decrease the failure risk of the ferroelectric film deposited on a piezoelectric substrate.

1. Introduction

Based on the ferroelectric domain switching and piezoelectric coupling, the application of ferroelectric film/substrate structures has been widely spread over many fields, typically the memory products. However, during long-term usage of ferroelectric film/substrate structures, their performance degradation induced by interfacial defects is unavoidable. Continuous polarization switching under a cyclic electric field causes the generation and accumulation of interfacial mismatch dislocations. The interfacial defects can inevitably lead to the internal friction and polarization fatigue. This concept was originally proposed by Merz and Anderson [1] in 1955. With the cumulative usage of film/substrate structures, the interfacial defects can proliferate with increasing usage cycles, leading to performance loss and even interface debonding. Lange et al. [2] discovered that the high cycle fatigue is a critical problem to design reliable ferroelectric actuators and sensors. The emergence of polarization fatigue can cause interfacial crack proliferation, and reduce the reliability and life span of smart devices.

The ferroelectric composite structure is usually driven by a high electric field, however the high electric field can induce a non-compatible strain field and a high voltage electrostatic field which may damage the structure. The low fracture toughness characteristic of ferroelectric materials has attracted great concern for the reliability and safety design [3]. Recently, Abdollahi et al. [4,5] simulated the conducting crack propagation of ferroelectric single crystal under pure electric field loading using extended phase-field model, and found that pure electric field loading can induce the crack tip charge accumulation which produces a high electric field

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Nomenclature

τ_{xz}	antiplane shear stress component along x axis
τ_{yz}	antiplane shear stress component along y axis
w	z axis displacement
φ	electric potential
D_x	x axis electric displacement component
D_y	y axis electric displacement component
$\mathbf{f}(z)$	complex potential function matrix
$\mathbf{F}(z)$	first order derivative of $\mathbf{f}(z)$ matrix
c_{44}	elastic constant
e_{15}	piezoelectric constant
$\varkappa_{11}$	dielectric constant
$\mathbf{G}_1$	generalized stiffness matrix of medium I
$\mathbf{G}_2$	generalized stiffness matrix of medium II
$\mathbf{G}$	generalized stiffness matrix
l	half width of domain a_2
L	crack interface
L'	continuous interface
t	arbitrary point on the interface
a_2	ferroelectric domain
$\mathbf{U}$	generalized displacement matrix
$\mathbf{U}^+$	generalized displacement function from region I to the interface
$\mathbf{U}^-$	generalized displacement function from region II to the interface
$\mathbf{\Sigma}_{xz}$	stress function matrix along x axis
$\mathbf{\Sigma}_{yz}$	stress function matrix along y axis
ω	disclination strength
$\boldsymbol{\omega}$	generalized disclination strength matrix
$\mathbf{F}_1^{\mathrm{film}}(z)$	thin film stress function
$\mathbf{P}_{\mathrm{ms}}$	concentrated loading
Q_{ms}	concentrated charge
$\mathbf{g}(z)$	complex potential function matrix
$\mathbf{g}_0(z)$	holomorphic complex potential function matrix
$\mathbf{A}(z)$	term concerning the singular points of z_1, z_2, $\overline{z_1}$ and $\overline{z_2}$
$\mathbf{G}(z_1)$	term concerning the singular point of z_1
$\mathbf{G}(z_2)$	term concerning the singular point of z_2
$\mathbf{G}(\overline{z_1})$	term concerning the singular point of $\overline{z_1}$
$\mathbf{G}(\overline{z_2})$	term concerning the singular point of $\overline{z_2}$
$\mathbf{G}(\infty)$	term concerning the singular point at infinity
$\mathbf{C}_0$	coefficient matrix
$\mathbf{C}_1$	coefficient matrix
K_{III}	SIF
K_{D0}	EDIF
l_0	reference length
K_{III0}	normalized SIF
K_{D0}	normalized EDIF
c_0	elastic constant ratio
k_0	dielectric constant ratio
e_0	piezoelectric constant ratio
a	half length of crack
$\mathbf{h}(z)$	complex potential function matrix
$\mathbf{F}_1^*(z)$	extension of the complex function matrix $\mathbf{F}_1(z)$
$\mathbf{F}_2^*(z)$	extension of complex function matrix $\mathbf{F}_2(z)$
S^+	region I
S^-	region II
$\mathbf{\Sigma}_{yz}^+$	generalized stress function from region I to the interface
$\mathbf{\Sigma}_{\mathbf{yz}}^-$	generalized stress function from region II to the interface
$\mathbf{F}_1^{\mathbf{P}_{\mathrm{ms}}}(z)$	stress function of a concentrated loading
P_{ms}	concentrated force

near the crack tip to further facilitate crack propagation. Wang [6,7] established the model of interface crack in piezoelectric materials with Maxwell stress and remanent polarization. The methods of the complex function and dual integral equations were developed to the piezoelectric fracture. The results demonstrate that the Maxwell stress and remanent polarization have obvious influences on both static and moving interface crack at special conditions. Zhang et al. [8] researched the crack propagation mechanism of the ferroelectric single crystal under pure electric field based on the analyses of the domain switching controlled by the crack tip field and the energy release rate. This reveals that the negative electric field causes the domain switching around the crack tip, providing the driving force for the crack propagation. Chen et al. [9] experimentally discovered the crack tip temperature of ferroelectric film/substrate materials is greatly elevated under the alternating electric loading with high frequency or large amplitude. With the increase of temperature, the energy barrier of domain switching near the crack tip drops down, and the SIF dramatically increases. This eventually leads to the unstable propagation of the crack; Conversely, the crack tip temperature increases slightly and become saturated rapidly under the low frequency or small amplitude alternating electric loading, in addition to this, the crack propagation was not observed. Fang et al. [10] researched the electric field induced fatigue crack growth in pre-cracked PZT ferroelectric ceramics, and found that the crack opening and closure under an alternating electric field are the major mechanisms of crack propagation. Furthermore, the frequency, waveform and amplitude ratio of the electric loading also have important effects on crack propagation. Xie et al. [11] studied the effect of dislocation toughening on the fatigue and fracture mechanism of ferroelectric film/substrate structures under piezoelectric coupling, and indicated that dislocations can significantly shield the I type cracks and enhance the SIF and EDIF. Above studies revealed the mechanism of the electromechanical coupling on the fracture of ferroelectric materials, but the effect of interfacial mismatch on the interfacial fracture of ferroelectric composites was not mentioned.

Liu et al. [12] discussed the effect of elastic mismatch between epitaxial layer and substrate on the critical thickness, and indicated that a softer substrate leads to a smaller critical thickness for misfit twinning. In addition, a Somigliana dislocation dipole model that can improve the calculation accuracy and efficiency was developed to determine the critical thickness of an epilayer for misfit twinning [13]. Fan et al. [14] investigated the effects of interfacial mismatch on failure behavior of bi-material interfaces and revealed that the effects of interfacial mismatch on fracture resistance and crack growth path are related to strength difference, and that the interaction between interfacial mismatch and strength difference determines failure behavior of the interfaces. Moridi et al. [15] studied the effect of lattice misfit strain on the residual stress of ferroelectric thin film system, analyzed the lattice mismatch as well as interfacial misfit dislocation in film/substrate structures in detail, and found that interfacial mismatch is the major cause of residual stress. The effects of the atomic level film debonding process and the interfacial mismatch on the lattice structure of the film/