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Modeling the fracture behavior of piezoelectric materials using a gradual polarization switching model

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ABSTRACT

Polarization switching experiments conducted on polycrystal piezoelectric materials indicate that the polarization switching is gradual (occurs over a range of applied electrical and mechanical loads). An empirical model that considers the gradual change in the polarization direction is proposed to capture the polarization switching phenomena and apply it to modeling the fracture behavior of piezoelectric materials. Changes in the dielectric constants (measured from a 90° polarization switching experiment) and the polarization direction are used to estimate the amount of domain switching for an applied electric field. To model polarization switching in a generalized state of stresses and electric fields, the applied electric field (during the experiment) is converted to the corresponding value of internal energy density causing polarization switching. Internal energy density is used as the parameter to estimate the amount of domain switching and the resulting gradual change in the polarization direction. The gradual polarization switching model computes changes in the material properties and spontaneous strain contributions (arising from crystal shape change in the switching domains) based on the current polarization direction. A finite element solution procedure that incorporates the gradual polarization switching model is developed and interfaced with ABAQUS. Stress–strain variations obtained from the compression experiments and FEA are compared for PZT-4 (Zr/Ti = 52/48) and PZT-5H (Zr/Ti = 53/47). The C(T) specimen that was used in Mode-I fracture experiments is analyzed with a slit crack assumption. Microscopic observations of the region near the crack tip of a C(T) fracture specimen is used to capture the actual crack geometry generated by the machining process. A finite element model with the actual crack geometry is used to investigate the influence of finite dimensions of the crack cavity on the size of the polarization switching zones in the vicinity of the crack tip and its effects on the opening stress and the stress intensity ahead of the crack tip.

1. Introduction

Macroscopic effects due to the polarization switching in polycrystal piezoelectric materials such as lead zirconate titanate (PZT) and lead lanthanum zirconate titanate (PLZT) from mechanical loads was studied by Cao and Evans (1993), Schaufele and Hardtl (1996), Calderon et al. (1997), Fang and Li (1999), Fan et al. (1999), and Chaplya and Carman (2000); from electrical loads by Fang and Li (1999), Wang et al. (1996), and Wan (2000); and from electromechanical loads by Lynch (1996) and Fett (2003). The thermoelectromechanical behavior of ferroelectric ceramics subjected to cyclic loads and high fields was studied by Mauck and Lynch (2003) and Weiland and Lynch (2003). Experimental studies on ferroelectric domain configurations and polarization switching at smaller scales were conducted using X-ray diffraction by Glazounov et al. (2001), atomic force acoustic microscopy and ultrasonic piezoelectric force microscopy by Rabe et al. (2002), scanning force microscopy by Saldana et al. (2003), and SEM by Saldana et al. (2004).

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Several phenomenological and micromechanical models have been proposed for modeling the ferroelectric material behavior. Chen et al. (1997) used a micromechanical approach and considered each single crystal to be composed of spherical domains to develop macroscopic constitutive relations. Huo and Jiang (1997) considered each grain to be made of multiple domains and used the difference in Gibbs free energy as the driving force for polarization switching to derive a constitutive law. Using a 1D treatment of the electromechanical behavior of a polarizable solid, Kim (1998) used a kinetic relation and a nucleation criterion to develop a continuum model for polarization reversals. The work criterion was proposed by Hwang et al. (1995) by considering each grain to be a single domain and that a ferroelectric switching results in a 90° or 180° change in the polarization direction, while a ferroelastic switching causes only a 90° polarization reorientation. It was used by Michelitsch and Kreher (1998) to model the nonlinear behavior under uniaxial electrical and mechanical loads. Kamlah and coworkers developed a phenomenological model to capture the nonlinear behavior of ferroelectric materials, beginning with an uniaxial treatment by Kamlah and Jiang (1999), Kamlah and Tsakmakis (1999) and a generalization to 3D by Kamlah and Bohle (2001). Chen and Lynch (1999) used a multiaxial constitutive law and considered the permittivity of the crack interior to demonstrate the effects of ferroelectric and ferroelastic switching through FEA of ferroelectric ceramics having elliptical cracks. Fan et al. (1999) observed the non 180° polarization switching to be a gradual process (initial softening and subsequent hardening) and used Maxwell chains arranged in parallel to simulate the irreversible strain. Fleck and coworkers considered domain wall motion to be analogous to slip system of dislocation plasticity and developed a nonlinear constitutive model to capture the behavior of a ferroelectric material for different load paths, as outlined by Huber et al. (1999) and a multiaxial constitutive model was presented in a simplified form by Huber et al. (2001) to make the computations faster. Cocks and McMeeking (1999) considered domain switching to be akin to plastic yielding and used kinematic hardening to characterize the change in shape of the switching surfaces and a 1D treatment was formulated. Landis (2002) extended the model for multiaxial loading states and higher computational speeds. McMeeking and Landis (2002) discussed the evolution of phenomenological models and developed a polarization switching model for multiaxial electromechanical loading of a polycrystal ferroelectric material. Li and Weng (1999) considered the thermodynamic driving and resisting forces during domain switching and determined the volume of switched domains, resulting overall strain, and polarization under applied electric field and stress. The theory developed was used to obtain the nonlinear stress–strain relation and depolarization of a poled PZT under an applied compressive stress. Li and Weng (2001) modeled the hysteresis behavior and the nonlinear stress–strain behavior under compressive stress in PLZT. Li and Weng (2004) modeled 180° domain switching in $BaTiO_3$ crystals. Li and Weng (2002) simulated the hysteresis behavior of PZT-51 and used the evolved material state to analyze the effects of applied axial or transverse compressive stress on the remnant polarization and coercive electric field. More recently, Su and Weng (2006) developed a two-level micromechanics theory, where a thermodynamics approach was used to determine the hysteresis behavior of the constituent grains and a self-consistent scheme was followed to translate the nonlinear behavior to the polycrystal level for modeling the behavior of PLZT. Kamlah et al. (2005) discussed a FEA approach, where the constitutive behavior of a polycrystal ferroelectric ceramic is computed using the technique developed by Huber et al. (1999) for multidomain single crystals. Wang et al. (2004) used a phase-field model and demonstrated the evolution of polarization switching, macroscale polarization, and strain changes under applied electromechanical loads.

Domain switching criteria based on work, energy, electric displacement (flux), and internal energy are popular in FEA and analytical work. A criteria based on work done (estimated using stresses and electric fields causing polarization switching and changes in spontaneous strains and polarization) during a switching of the polarization direction of a single domain was proposed by Hwang et al. (1995). The work criteria was modified by Jiang and Sun (1998) to include the effect of spontaneous, as well as induced changes in strains and electric displacements (arising from changes in piezoelectric property) that accompany the switching of domains. Sun and Chang (2000) proposed further modifications to the work criterion by using average values of stresses and electric fields (observed in polarization switching experiments) to compute the work required for polarization switching. Chen and Lynch (1998) developed a micromechanics model which considers the interaction between grains and found that they have an influence on the hysteresis behavior of PLZT under a mechanical load. Lu et al. (1999) used a distribution of domain orientations and the difference in Gibbs energy as the driving force for polarization switching to capture the variations in strains and electric displacements observed during hysteresis experiments on PZT-51 and PLZT. A critical value of electric displacement was proposed as a criterion for polarization switching by Fontinich and Carman (2000) in their study of strains and stresses arising from polarization switching and Fontinich and Carman (2002) modeled the nonlinear behavior using a distribution of domains poled in different directions. An internal energy density criterion was proposed by Sun and Achuthan (2004) and was found to predict the experimentally observed 90° and 180° polarization switching behavior more accurately than other criteria. Kalyanam et al. (2002) incorporated it in a FEA procedure and quantified the effects of polarization switching on the fracture toughness of C(T) specimens of PZT-4. A critical value of work, energy or electric displacement is appropriate when a domain switches completely (all crystals in the domain switch at one instant). In reality, the nonlinearities present in a polycrystal piezoelectric material cause the domains within a grain to switch gradually. The presence of a large number of grains and multiple domains within each grain require the modeling approach to consider each domain independently and its polarization direction be updated