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# Rate-dependent electro-mechanical coupling response of ferroelectric materials: A finite element formulation

Amir Sohrabi, Anastasia Muliana *

*Mechanical Engineering Department, Texas A&M University, United States*

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ABSTRACT

This paper presents a three-dimensional (3D) constitutive model for predicting nonlinear polarization and electro-mechanical strain responses of ferroelectric materials subject to various histories of electric fields and mechanical stresses. The electro-mechanical coupling constants are expressed as functions of a polarization state and it is assumed that in absence of the polarization, the material does not exhibit electro-mechanical coupling response. The polarization model due to an electric field input is additively decomposed into time-dependent reversible and irreversible parts. The model also incorporates the effect of compressive stresses on the polarization response. Thus, the constitutive model is capable of incorporating the effect of loading rates, mechanical stresses, and electric fields on the overall hysteretic electro-mechanical and polarization switching response of ferroelectric materials. The constitutive model is implemented in a continuum 3D finite element in order to perform rate-dependent electro-mechanical coupling analyses of smart structures. The experimental data on the polarization switching and hysteretic butterfly strain responses of lead zirconate titanate (PZT) reported by Fang and Li (1999) are used to validate the constitutive model. Parametric studies are also conducted to examine the effect of loading rates and coupled electro-mechanical boundary conditions on the overall performance of PZT. Finally, FE analyses are performed to simulate shape changing in smart composite structures.

## 1. Introduction

Ferroelectric materials, such as lead zirconate titanate (PZT) and polyvinylidene fluoride (PVDF), have been widely used in sensor, actuator, and energy conversion devices, where they are subjected to various histories of electro-mechanical stimuli. Several experimental studies have been conducted on understanding the response of ferroelectric materials under cyclic electric fields with amplitudes higher than the coercive electric field limits. Under such loading conditions, ferroelectric materials exhibit polarization switching, e.g., Schmidt (1981), Gookin et al. (1984) and Fang and Li (1999). It was also shown that compressive stresses that are applied along the poling axis of the ferroelectric materials could induce depolarization of the poled ferroelectric materials (Lynch (1996), Chen and Lynch (1998) and Fang and Li (1999)). Fang and Li (1999) experimentally studied changes in the polarization and butterfly strain loops of a PZT specimen under a cyclic electric field input. After several cycles, the saturated polarization response converges to a constant value, which is slightly smaller than the one measured in the first cycle. An experimental study on a polarized PZT specimen under cyclic electric fields with the maximum amplitude of 85% of the coercive electric field of the PZT, reported by Crawley and Anderson (1990), shows nonlinear electro-mechanical response. They observed that the effects of creep and loading rate on the piezoelectric constant were more significant at larger strains and lower frequencies. The electrical and mechanical responses of ferroelectric materials are time and frequency dependent, which were

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* Corresponding author.
*E-mail address:* amuliana@tamu.edu (A. Muliana).

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experimentally shown by Fett and Thun (1998), Schaeufele and Haerdtl (1996), Zhou and Kamlah (2005), Zhou and Kamlah (2006) and Ben Atitallah et al. (2010), among others. Zhou and Kamlah (2005), Zhou and Kamlah (2006) showed the creep response in a soft PZT under static electric fields and compressive stresses, which were more pronounced at higher stresses and at electric fields near the coercive electric field.

There have been constitutive models developed to predict nonlinear electro-mechanical behaviors of ferroelectric materials, which can be classified as phenomenological (macroscopic) models based on continuum mechanics approach and micromechanics based models that incorporate the microstructural morphologies of the materials. In an analogy to rate-independent plasticity theory, macroscopic constitutive models have been formulated for predicting polarization switching response in ferroelectric materials due to electric field inputs. The strains and electric displacements are additively decomposed into reversible and irreversible components. Examples of these macroscopic models can be found in Bassiouny et al. (1988a) and Bassiouny et al. (1988b), Bassiouny and Maugin (1988a), Huang and Tiersten (1998a,b), Kamlah and Tsakmakis (1999), Linnemann et al. (2009). Recently, Muliana (2011) presented a phenomenological model for time-dependent polarization and electro-mechanical strain responses of ferroelectric materials subject to various histories of electric fields. The model is capable of predicting the polarization switching response of piezoelectric ceramics at various rates of electric field inputs. Massalas et al. (1994) and Chen (2009) presented nonlinear electro-mechanical constitutive equations for materials with memory-dependent (viz. viscoelastic materials). They also incorporate the dissipation of energy due to the viscoelastic effect, which is converted into heat. The macroscopic response of materials depends strongly upon their microstructural response, which occurs at various length scales. Microscopically motivated constitutive models that take into account polarization response of each crystal in predicting the overall nonlinear electro-mechanical response of ferroelectric materials can improve our understanding on the nonlinear behavior of ferroelectric materials. Examples of the micromechanics based constitutive models for polarization switching in ferroelectric materials can be found in Chen and Lynch (1998), Fan et al. (1999), Li and Weng (1999, 2001), Smith et al. (2003, 2006), Su and Landis (2007).

Finite element (FE) methods have been used for analyzing the electro-mechanical response, including the hysteretic polarization switching response, of structures consisting of conductive and ferroelectric materials mainly for *time* (*rate*) – *independent* behavior, e.g. Kamlah and Bohle (2001), Landis (2002), Zheng et al. (2003), Li and Fang (2004), Zhang and Bhattacharya (2005), Klinkel (2006), Wang and Kamlah (2009), Linnemann et al. (2009), Klinkel and Wagner, 2006, and Muliana and Lin (2011). In the above FE formulations, macroscopic constitutive models are used for the electro-mechanical coupling response of piezoelectric and ferroelectric materials. Zheng et al. (2003) presented incremental and iterative solutions for problems involving polarization switching due to high electric field and heat generation from the dissipation of energy during the domain reversal process. FE methods that also include the *time* (*rate*) – *dependent* effects are currently limited. Kim and Jiang (2002) presented FE algorithm for simulating macroscopic polarization and strain responses in ferroelectric materials undergoing domain switching. The macroscopic electro-mechanical constitutive models include the effect of different polar axes in the crystallites, whose contributions are quantified by mass fractions. The macroscopic polarization, strains and electro-mechanical properties are obtained using the weighted average of their microstructural configurations through the mass fractions. They also defined the functions for the rate of change of the mass fractions, which allow for incorporating rate-dependent loadings.

Experimental studies show that the electro-mechanical response of ferroelectric materials is *time*- (*and rate*-) *dependent* when subjected to electric fields and mechanical loadings. The electro-mechanical response of ferroelectric materials also depends strongly upon the applied electric fields and mechanical stresses. This study presents a three-dimensional (3D) rate-dependent electro-mechanical coupling constitutive model for ferroelectric materials undergoing various histories of mechanical stress and electric field. The constitutive model is derived for materials undergoing small deformation gradients which are suitable for ferroelectric ceramics. The constitutive model is capable of predicting the overall electro-mechanical and polarization switching behaviors of the ferroelectric materials. This study concerns with the polarization switching response due to application of electric fields and examines the effect of mechanical stresses during the polarization switching. It is noted high stresses can also induce polarization switching in ferroelectric materials; however, stress induced polarization switching is not being considered in this manuscript. The polarization due to an electric field input is additively decomposed into the time-dependent reversible and irreversible parts, in which the irreversible part is due to the polarization switching process. The electro-mechanical coupling material constants are taken as nonlinear functions of a polarization state and in absence of the polarization the electro-mechanical coupling constants would vanish. The model also assumes that the coercive electric field of the ferroelectric material depends on the mechanical stress. This constitutive model is implemented in 3D continuum element and used to perform structural analyses. Two scales of integration algorithms based on recursive and iterative schemes are formulated at the constitutive material and finite element levels. The manuscript is organized as follows. Section 2 presents the time-dependent electro-mechanical constitutive model followed by its FE implementation in the three-dimensional continuum elements in Section 3. Section 4 presents numerical examples of the time-dependent nonlinear electro-mechanical response of ferroelectric structural components. Section 5 is dedicated to concluding remarks.