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Finite element analysis of switching domains using ferroelectric and ferroelastic micromechanical model for single crystal piezoceramics

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ABSTRACT

Here, the domain switching in a ferroelectric and ferroelastic single crystal subjected to electrical, electromechanical, and mechanical loading condition is studied. An isoparametric 3D electromechanical hexahedral finite element introducing the micromechanical constitutive law for domain switching is proposed to investigate the non-linear response of single crystal piezoceramics. The micromechanical model considered here is based on thermodynamic approach and internal variables, accounting for the electromechanical interaction energy between the domains. The volume fractions of six distinct uni-axial variants are treated as the internal variables to describe the microscopic state of the material at any given loading level. Furthermore, the formulation includes a realistic phase transition from a cubic unit cell to tetragonal one in the single crystal piezoceramics under the application of external load. The non-linear electromechanical constitutive equations obtained are solved using an implicit integration technique employing the return-mapping algorithm. The model developed here is tested for its applicability considering variety of benchmarks, and it brings out the behaviour of piezoceramic materials as observed in experimental studies.The hexahedral finite element presented is also implemented in the commercial finite element code Abaqus via the User Element subroutine.

1. Introduction

Piezoelectric materials have a unique electromechanical coupling behaviour that serves as an essential aspect of smart material applications [1]. The sensor and actuator technologies currently involve complex loadings and geometries to enhance the actuation and sensing capabilities of piezoelectric actuators and sensors, respectively. The response of the piezoelectric materials is in general linear when they are subjected to low electric fields or mechanical stresses. However, they may exhibit non-linear behaviour under high electric fields or mechanical stress [2,3]. Kamlah et al. [4] have studied the characteristics of a polycrystalline piezoceramic using a multi-domain single crystal switching model and finite element approach. The two dimensional model considered here deals with the plane strain condition that may limit its applications when the piezoceramics are subjected to pure mechanical loading. The domain nucleation and propagation of domain walls in the presence of defect in the piezoceramic plates have been investigated in the literature [5]. The effect of uniaxial stress on the coupling properties of various piezoelectric ceramics and single crystals has been examined in Refs. [6,7]. Most of these studies show that the linear constitutive law may not be sufficient to explain the behaviour of piezoceramics under complex loading situations. Experimental studies have been conducted to understand the behaviour of piezoelectric materials and reported in the literature [8–11]. They have highlighted the existence of the non-linear response of piezoelectric materials. Thus, it necessitates for the development of realistic model in predicting the actual characteristics of the piezoceramic material under these circumstances.

Two types of non-linear constitutive models, namely, phenomenological (macroscopic) and microscopic models are proposed in the literature to predicting the response of piezoelectric materials under high electrical and/or mechanical loadings. Phenomenological models are generally developed based on internal variables at any given loading level and the evaluation of these internal variables is determined by the kinetic equations. Also, they require a few internal variables to estimate the macroscopic behaviour when compared to those of micromechanical models [12–15]. Although the macroscopic approach predicts the

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characteristics of ferroelectric single crystal qualitatively while comparing with experimental results, it may not capture the microscopic reorientation of domains that causes smooth transition during domain switching [16]. Attempt is also made to enhance the phenomenological model with domain switching for ferroelectric single crystals under electromechanical loading, incorporating different energy dissipation, and neglecting the grain to grain interaction [17].

Models that are established introducing the microscopic mechanism of domain switching are denoted as the micromechanical models. These models are generated assuming the description of the material at the ferroelectric and ferroelastic domain length scale and averaging over a large number of oriented crystallites to reproduce the behaviour of polycrystals. These models yield a better physical insight into the material response, and they can bring out the microstructural variations in a better way than the phenomenological models [18,19]. Hwang et al. [20] have examined the material behaviour using micromechanical model with the domain switching process in ferroelectrics under the combined electrical and mechanical load. In this model, the crystal is assumed to be tetragonal in shape with randomly oriented crystals/grains and the characteristics is evaluated by averaging the responses of several single crystals. Switching criterion based on various energy criteria such as Gibbs energy [21], potential energy [22], internal energy density [23] and electric displacement [24] have been employed to determine the onset of domain switching. A two-step switching criterion was proposed based on domain switching mechanisms that divide the 180° switching into two 90° switching [25]. Huber et al. [26] considered the existence of all domains in a single crystal and dealt with the incremental switching coupled with self-consistent method while carrying out the response of the polycrystal. This model brings out the influence of domain wall motion with a gradual change in remnant strain and polarization. However, this model requires in general a high computational time and more so with the increase in the complexity of the problem. Elhadrouz et al. [27] have developed a micromechanical model including the influences of the polarization and strain incompatibilities due to domain switching. The numerical simulation is performed considering the mechanical loading but it has not shown the efficacy of the model in predicting the behaviour of piezoceramics under electrical and electromechanical loading cases. Also, this formulation did not interface with the scale transition technique in order to describe the electromechanical behaviour of polycrystalline aggregate. Jayabal et al. [28] proposed a three-dimensional micromechanical model for the evaluation of non-linear dissipative effects in the polycrystal ferroelectrics by applying the constraint imposed by the surrounding grains on a subgrain at its boundary during domain switching. However, it is unable to bring out the smooth transition during domain switching as observed in experimental work.

Numerical method like finite element approach is mostly employed in designing reliable piezoceramic structures for various applications [29,30]. A 3D electromechanical hexahedral 8-noded element has been developed [31,32] using 3D phenomenological constitutive laws and electromechanical coupling effects. Ref. [33] dealt with the classical shell element and it may not be suitable for studying the piezoelectric structures dominated by the longitudinal d_{33} effect as the thickness variation is not considered. A ferroelectric and ferroelastic 3D hexahedral curvilinear finite element in conjunction with a 3D phenomenological model is introduced to examine the macroscopic behaviour of piezoceramic structures in Ref. [29]. Zheng et al. [34] have outlined in obtaining different alternative methods assuming the domain switching criteria based on the variational formulation for different parings of independent variables [i.e. (ϵ, E), (σ, D), (ϵ, D) and (σ, E)]. Sohrabi and Muliana [35] developed a rate-dependent model to understand the electro-mechanical coupling response of ferroelectrics. Numerical and experimental analysis of electromechanical coupling of a cantilever beam with piezoelectric patches is carried out in Ref. [36]. A polygonal finite-element constitutive model has been formulated to understand the electromechanical behaviour of piezoceramics and it does not address the domain evolution due to micro-crack initiation in piezoelectric structures [37]. A physics based micro non-linear model for the magneto-electric composites is addressed by Avakian et al. [38] assuming the non-linearity in ferroelectric phase and linear magnetostrictive constituents. This study shows the importance of the non-linear modeling for the simulation of a poling process and the prediction of Magneto-Electrical (ME) coupling, and for bringing out the influences of residual stress and polarization scattering. However, it has some limitations due to the omission of the non-linear ferromagnetic phase and the evaluation of ferroelectric domain with the presence of defects.

It is observed from these discussions on the available work pertaining to the different constitutive models and their implementation in numerical method that, among researchers, there is a growing appreciation of importance of developing better models for the evolution of the accurate prediction of the global/local behaviours of piezoelectric material under various loading situations and resulting in computationally less expensive. Furthermore, it may be worthwhile to revisit, in particular, the available micromechanical models for the analysis of switching domain at grain and polycrystalline levels and to develop an improved formulation by realistically representing the constitutive law through the modeling of domain switching, the field distribution within the grains and the imposition of the associated boundary constrains, an appropriate numerical technique, and integration of the materials model with the finite element procedure, etc.

In the present work, an improved constitutive model based on micromechanical approach is developed by extending the earlier work of one of the present authors [27], and is also focused on improving the numerical aspects of the developed model and its implementation in an electromechanical finite element [33]. This formulation is developed for modeling the behaviour of polycrystalline piezoelectric materials, the field distribution inside the grains and also in describing the domain wall motions inside grains. The implicit integration of the non-linear constitutive equations is carried out, based on return-mapping algorithm. The proposed micromechanical model is implemented within a 3D electromechanical 8-noded hexahedral element with electrical and mechanical degrees of freedom, named as H8F and this element is tested for its applicability considering wide range of benchmarks and compared with the available studies in the literature. Finally, this element is implemented into the Abaqus code via subroutine user element (UEL).

The present article is divided into six sections. In the following section, the variational formulation of the piezoelectric problem is briefly recalled. The 3D micromechanical ferroelectric and ferroelastic constitutive law and its local numerical integration are presented in Section 3. 3D electromechanical curvilinear element presentation and its implementation into Abaqus are discussed in Section 4. In Section 5, the ferroelectric and ferroelastic benchmarks are considered to validate the developed model and FE analysis of switching domains and the domain interface motion. Finally the paper concludes with a summary in Section 6.

2. Variational formulation for a piezoelectric system

Consider a piezoelectric domain bounded by the surface S and with volume V as shown in Fig. 1. Based on Newton's second law