A ferroelectric and ferroelastic 3D hexahedral curvilinear finite element

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An isoparametric 3D electromechanical hexahedral finite element integrating a 3D phenomenological ferroelectric and ferroelastic constitutive law for domain switching effects is proposed. The model presents two internal variables which are the ferroelectric polarization (related to the electric field) and the ferroelastic strain (related to the mechanical stress). An implicit integration technique of the constitutive equations based on the return-mapping algorithm is developed. The mechanical strain tensor and the electric field vector are expressed in a curvilinear coordinate system in order to handle the transverse isotropy behavior of ferroelectric ceramics. The hexahedral finite element is implemented into the commercial finite element code Abaqus® via the subroutine user element. Some linear (piezoelectric) and non-linear (ferroelectric and ferroelastic) benchmarks are considered as validation tests.

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1. Introduction

Piezoelectric ceramics like barium titanate (BaTiO3) and lead zirconate titanate (PZT), defined as poled ferroelectric ones, play an important role in advanced sensor and actuator applications thanks to their well-known piezoelectric coupling effects between electric and mechanical fields (Ikeda, 1996). Nowadays, many piezoelectric applications involve severe loadings and complicated geometries to enhance, for example, the mechanical displacement of piezoelectric actuators. In this case, the assumption of linear behavior is no longer sufficient to reliably analyze the stress and electric field states in piezoelectric devices. In fact, when subjected to high electromechanical loadings, piezoceramics exhibit a non linear behavior due to ferroelectric and ferroelastic switchings caused by an electric field and a mechanical stress, respectively (Kamlah and Böhle, 2001; Elhadrouz et al., 2005).

To take into account this non linear behavior, some microscopically motivated material models have been proposed in Chen and Lynch (1998), Hwang et al. (1998), Kamlah et al. (2005). These models describe the constitutive behavior of single crystals and an averaging over a large number of oriented crystallites should be considered to obtain the polycrystalline ceramic behavior. Consequently, a considerable number of internal variables is needed as switching criterion is written for each crystal of the ceramic. Consequently, a considerable number of internal variables is needed as switching criterion is written for each crystal of the ceramic. In order to reduce the number of internal variables, some phenomenological macroscopic models have been proposed. In this case, a thermodynamically sound model has been proposed in Bassouiny and Maugin (1988, 1989). The main idea has been the additive decomposition of the strain and electric polarization into a reversible part and a remanent part as in thermo–elasto–plasticity. In this case, the irreversible polarization and the irreversible strain can be used as internal variables to describe the loading history of piezoelectric compounds. On the basis of this concept, some models have been developed in Kamlah and Tsakmakis (1999), Cocks and McMeeking (1999), Kamlah and Böhle (2001), McMeeking and Landis (2002), Landis (2002), Elhadrouz et al. (2005). In Kamlah and Tsakmakis (1999, 2001), the irreversible strain tensor was additively decomposed into two parts. One remanent part appears due to the alignment of the domains along the applied electric field direction and the second one is caused by the mechanical stress. A one-to-one relation between the first remanent strain, named ferroelectric strain, and the irreversible polarization was assumed. This model is able to simulate all ferroelectric and ferroelastic hysteresis loops including mechanical depolarization effects shown experimentally in ferroelectric ceramics. Besides, it was shown in Kamlah and Böhle (2001) that the proposed model is able to detect the dielectric hysteresis and butterfly loops “crushing” occurring under the application of a high constant compressive stress as shown in Lynch (1996).

In Elhadrouz et al. (2005), the general assumptions made in Kamlah and Böhle (2001) were considered. The main originality concerned the additive decomposition of the remanent polarization into a first part caused by the electric field, named ferroelectric polarization, and a second one caused by the mechanical stress. The model is also able to predict ferroelectric and ferroelastic hysteresis loops as well as the mechanical depolarization. Nevertheless, it was not shown whether the model is capable or not to detect the dielectric hysteresis and butterfly “crushing” under high compression stresses.