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Three-dimensional finite elements with embedded strong discontinuities to model failure in electromechanical coupled materials

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ABSTRACT

This paper presents new finite elements with embedded strong discontinuities to model failure in three dimensional electromechanical coupled materials. Following the strong discontinuity approach for plane electromechanical problems, the coupled boundary value problem is decomposed into a continuous global part and into a discontinuous local part where strong discontinuities in the displacement field and electric potential are introduced. Those are incorporated into general three-dimensional brick finite elements through nine mechanical separation modes and three new electrical separation modes. All the local enhanced parameters related to those modes can be statically condensed out on the element level, yielding a computationally efficient framework to model failure in electromechanical coupled materials. Impermeable electric boundary conditions are assumed along the strong discontinuities. Their initiation and orientation is detected through a configurational force driven failure criterion. A marching cubes based crack propagation concept is used to obtain smooth failure surfaces in the three dimensional problems of interest. Several representative numerical simulations are included and compared with experimental results of failure in piezoelectric ceramics to outline the performance of the new finite elements.

1. Introduction

Electromechanical coupled materials play an important role as actuators, transducers or sensors in smart systems. Extensive research on their electromechanical properties has been performed over the years resulting in general frameworks and reviews of their phenomenological and micromechanical motivated constitutive response [1–5]. Their high ultimate strength and extremely low fracture energy makes those materials prone to develop cracks, affecting their mechanical properties like durability or strength. Numerous theoretical [6–11] and experimental [12–14] studies on the failure characteristics of, in particular, piezoelectric ceramics are available in the literature. In this work, a computational framework is proposed to model the onset and propagation of failure in three-dimensional electromechanical coupled materials.

A large number of numerical techniques have been developed to model purely mechanical solids at failure such as cohesive finite element formulations [15,16], adaptive remeshing techniques [17–21], phase-field models [22–30], the extended

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finite element method [31–34], or the embedded finite element method [35–40]. Their extensions to model fracture in electromechanical coupled problems though is only in its infancy [41–50] and serves as the main motivation for this work.

In particular, we consider the *embedded finite element formulation*, which introduces enhanced local kinematic parameters to describe failure zones such as cracks or shear bands through strong discontinuities in the displacement field for purely mechanical problems. This approach, originally developed in [35] is extended in [51,52] to three dimensions, in [53,54] to porous media, in [55–57] to structural problems such as beams and plates, in [58–61] to account for higher order kinematic approximations of the displacement field within the two dimensional (2D) and three dimensional (3D) continuum setting, in [62,63] to dynamic fracture, in [64] to multiple levels, and in [43–45] to 2D electromechanical coupled materials. Those latter works serve as the starting point for the extension to model failure in 3D electromechanical coupled problems in this work.

Following [43], the overall electromechanical boundary value problem (BVP) is decomposed in this work into a continuous global problem, treated as the standard electromechanical BVP, and a discontinuous local problem, where jumps in the displacement field and electric potential are incorporated along the strong discontinuities. The decomposition of the method into a global and a local part results in an efficient numerical implementation by enhancing the standard displacement based, mixed, enhanced three-dimensional brick finite elements with local parameters carrying the information of jumps in the displacement field and electric potential. Those enhanced parameters, which all can be statically condensed out on the element level therefore leading to a computational efficient formulation, are associated with three newly introduced electrical separation modes and the nine mechanical separation modes proposed in [60] with a slight modification of the rotation mode around the normal of the failure surface by an in-plane shear mode in [61]. The smoothness and continuity of the final failure surfaces is ensured in this work through the incorporation of the marching cubes based crack propagation concept proposed in [61] for purely mechanical problems.

One particular challenge for the modeling of failure in electromechanical coupled materials lies in the detection of the onset of failure and in the determination of the failure zone orientation. Existing failure criteria are based on the total energy release rate [65,8,66], the mechanical energy release rate [12], the local energy release rate [9,67], the strain energy density [68], the mechanical crack tip opening [69], or are based on a simplified form of the loss of ellipticity condition [43], among others. Extending the proposed treatment in [43] for plane problems to the 3D setting in this work has though resulted in an unsatisfactory performance with non-physical fracture zone orientations. It is for this reason, that we pursue a different strategy in this work through the application of a configurational force driven failure criterion based on the electromechanical coupled Eshelby stress tensor [70–73], where the numerical implementation proposed in [20,21,74–76] is adopted. As in [42], only the mechanical contribution of the electromechanical coupled configurational forces is considered as failure criterion in this work.

The paper is organized as follows. Section 2 summarizes the classical electromechanical BVP within the continuum setting in Section 2.1 and the discrete setting in Section 2.2. The incorporation of strong discontinuities in 3D electromechanical coupled solids is outlined in Section 3. In particular, the incorporation of strong discontinuities in the electric potential is outlined in detail within the continuum setting in Section 3.1 and within the discrete setting in Section 3.2. The configurational force based failure criterion and crack propagation concept is discussed in Section 3.3. Section 4 describes the design of new finite elements through the development of three new electrical separation modes avoiding otherwise appearing locking phenomena in the 3D brick finite elements. The performance of the new finite elements is outlined in Section 5 based on three academic single element tests and two realistic tests in the form of a compact tension test and a three point bending test with different notch locations. The latter two problems allow us to validate the performance of the newly developed finite elements through a qualitative and quantitative comparison with experimental results available in the literature [12]. Several concluding remarks are given in Section 6.

2. The standard electromechanical BVP

This section briefly summarizes the global governing equations of the classical electromechanical BVP within the infinitesimal range of interest in this work. We separately discuss the continuum and the discrete framework in Sections 2.1 and 2.2, respectively. Failure is not accounted for in this section with its treatment through the incorporation of strong discontinuities postponed to Section 3.

2.1. The electromechanical BVP in the continuum setting

Let $\mathcal{B} \subset \mathbb{R}^3$ be a electromechanical coupled solid with the primary unknowns of the mechanical displacement $\boldsymbol{u}$ and the electric potential φ. The infinitesimal strain tensor $\boldsymbol{\varepsilon}$ and the electric field $\boldsymbol{e}$ at material points $\boldsymbol{x} \in \mathcal{B}$ are then defined by

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \text{sym}[\nabla \boldsymbol{u}] = \frac{1}{2}[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T] \quad \text{and} \quad \boldsymbol{e}(\varphi) = -\nabla \varphi \tag{1}$$

in terms of the gradient operator ∇ with respect to the coordinate $\boldsymbol{x}$. For piezoelectric ceramics, the corresponding stress tensor $\boldsymbol{\sigma}$ and the electric displacement field $\boldsymbol{d}$ follow as

$$\boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\varepsilon} - \mathbb{h}^T \boldsymbol{e} \quad \text{and} \quad \boldsymbol{d} = \mathbb{h}\boldsymbol{\varepsilon} + \mathbb{b}\boldsymbol{e} \tag{2}$$