MIXED FINITE ELEMENT METHOD FOR FRACTURE MODELING OF PIEZO- AND FERROELECTRIC MATERIALS WITH STRAIN GRADIENTS (FLEXOELECTRICITY)

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Abstract

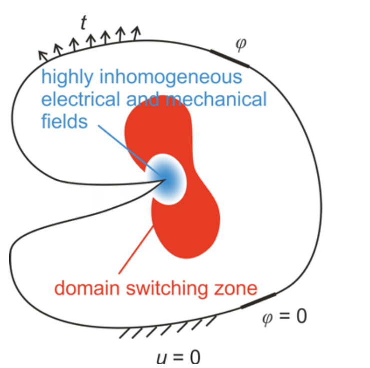
Following the continuous miniaturization of the microelectromechanical systems (MEMS), a size-dependent phenomenon of flexoelectricity starts to play an essential role at the micro- and nanoscale. Direct flexoelectricity is an electromechanical coupling of strain gradients, which are inversely proportional to the length scale, and electric field. Due to the application of strain gradients, the centrosymmetry of the unit cells is broken, allowing a wider choice of dielectrics to be used in applications. In the proposed research, the nonlinear ferroelectric material behavior is further enhanced with strain gradients and applied to fracture problems with naturally occurring gradients of electromechanical fields near the crack tip. Or in another way, it is the incorporation of the remanent strains and polarization into the flexoelectric formulation. Our solution demonstrates the strong influence of the gradients on the ferroelectric domain switching behavior, leading to modified electromechanical fields close to the crack tip compared to the well-known ferroelectric problems.

1. Introduction

Ferroelectricity has been studied for a couple of decades, and many important fracture mechanics problems were solved, e.g., the numerical modeling of polycrystalline ferroelectric ceramics fracture under monotonic and cyclic mechanical or electric loading [1]. However, the incorporation of strain gradients into nonlinear ferroelectric formulations is unknown to the authors. In the case of flexoelectricity in dielectric and piezoelectric materials, numerical modeling using collocation-based mixed FEM with second-order elements was proposed recently [2]. Additionally, two new numerically robust mixed finite elements were developed and used to perform numerical simulations of edge-cracked panels in order to highlight the mutual interactions of piezoelectricity and flexoelectricity [3]. In the very recent time, the research progressed to incorporate ferroelectricity phenomena [4].

2. Results

Numerical simulations of Griffith crack with the proposed user elements [3] illustrate the influence of activating flexoelectricity in piezoelectric solids. It is observed that there is a massive change in the profile of electric potential generated in MEMS when strain-gradient elasticity is activated, namely, there is a mutual cancellation or superposition of the electric potential profiles depending on the polarity of the piezoelectric material. The contribution of piezoelectricity becomes significant, starting from the structural size of hundreds of nanometers or larger. It is observed that mutual interactions of piezoelectricity and flexoelectricity result in tremendous electromechanical activity in the vicinity of the crack tip. The ferroelectric domain reorientation is activated even well below the coercive electric field [4]. The domain-switching pattern is influenced as well. The mutual coupling and interplay between the electromechanical coupling due to the non-centrosymmetric structure of tetragonal unit cells of piezo-/ferroelectric materials and flexoelectricity contribution due to gradient terms become very complicated. Application to the fracture problems shows the need to revise the commonly used domain switching criterion along with the traditional fracture criteria.



Interplay between the ferroelectric domain switching zone and region of gradient terms dominance

3. Conclusions

The current research introduces the first steps towards nonlinear ferroelectric fracture mechanics simulations advanced with strain gradients, and develops "ferroelectricity-flexoelectricity" numerical setup. For this purpose, recently developed mixed FE for flexoelectric solids is further extended with micromechanical domain switching model. The results of our simulations highlight the importance of electromechanical gradients' contribution in the domain switching active regions.

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