

A CONDENSED APPROACH TO MODELING AND ANALYSIS OF FERROELECTRIC PZT AT THE MORPHOTROPIC PHASE BOUNDARY

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Key words: *Ferroelectrics, grain interaction, residual stresses, hysteresis loops, tetragonal and rhombohedral unit cells*

Ferroelectric materials as components of smart structures are widely used as bulk material in actuators or sensors and are constituents of microelectromechanical systems. The material behavior has been well investigated during the past decades. For its simulation, the finite element method is usually used. However, the FEM is a very complex and expensive method. Also, it is not necessary to solve a boundary value problem if just hysteresis loops or other bulk properties are to be investigated. On the other hand, the investigation of smooth hysteresis loops or residual stresses due to strain or charge incompatibilities requires the modeling of a polycrystalline material with complex grain interactions.

In the paper a condensed model for ferroelectric solids with tetragonal and rhombohedral unit cells is presented. It incorporates the above outlined issues without being implemented within the framework of a spacial discretization scheme. The approach is microelectromechanically and physically motivated considering discrete switching processes on the level of unit cells and quasi-continuous evolution of inelastic fields on the domain wall level. To calculate multiple grain interactions an averaging technique is applied. Hysteresis loops are simulated for pure electric and electromechanical loading demonstrating e.g. the influence of a compressive preload on the poling and stress-strain behavior. Further, residual stresses are calculated as a result of switching processes and interactions between statistically arranged crystallites. These stresses and some hysteresis loops are compared to Finite Element calculations demonstrating the potential of the condensed approach. Also, a simple micromechanical damage model is presented combining ferroelectric domain switching and micro crack growth.