IOWA STATE UNIVERSITY

Materials Science & Engineering Department

Jingyi Zhang

Final Oral Examination
MS Student with Wei Hong

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"Phase-field model simulation of ferroelectric/antiferroelectric microstructure evolution under multiphysics loading"

Ferroelectric (FE) and closely related antiferroelectric (AFE) materials have unique electromechanical properties that promote various applications in the area of capacitors, sensors, generators (FE) and high density energy storage (AFE). However, reliability issues changes its paradigms and requires guidance from detailed mechanism theory as the materials applications are pushed for better performance. A host of modeling work were dedicated to study the macro-structural behavior and microstructural evolution in FE and AFE material under various conditions.

This thesis is focused on direct observation of domain evolution under multiphysics loading for both FE and AFE material. Landau-Devonshire time-dependent phase field models were built for both materials, working models were built in a finite element analysis approach and FE/AFE behavior under multiphysics loading were systematically studied. Materials structure of polycrystal materials including grain orientation, grain boundary, defects and materials texture were tested for their effect on hysteresis and switched domain growth. Detailed microstructure development in domain switching and alignment was directly observed in this simulation.

In FE simulation, dagger-shape 90 degree switched domain was observed at preexisting crack tip under pure mechanical loading, and blocking effect of the growth of switched domain from grain misorientation and/or grain boundaries was observed. AFE model was developed using two sublattice theory, and this model was used to investigate the mechanism of energy efficiency increase in self-confined samples. Consistent results with experimental data was found and provided evidence that origin of energy density increase rise from inner compression field, fringe leak and uneven defects distribution. Texture of material was also considered and developed as a vector field in our FE and AFE models. The simulation gave quantatively results for the well-recognized irreversible strain in AFE virgin ceramics during the first poling process. The texture field shows a shielding zone under mechanical loading around existing crack tip.