# Developing Electromechanically Coupled Computational Methods for Piezoelectrics/Ferroelectrics at Multiscale

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We present research results of the multi-scale computational methods for ferroelectrics/piezoelectrics developed at our group in the past decade. In the macroscopic methods, we introduce the linear/nonlinear finite element methods and the meshless method for linear piezoelectrics. The rescaling technique in the linear FEM and the domain switching instability problem in nonlinear FEM were specially addressed. In the mesoscopic methods, the conventional phase field models (PFM) and the optimization-based computational mechanics methods were both presented and the domain pattern evolution in single crystals and domain texture evolution in polycrystals were obtained. In the atomic-level methods, we employed the first-principles method to investigate the topological polarization and flexoelectricity response and adopted the modified electromechanical coupled molecular dynamics method to address the size effect and surface effect in ferroelectric thin films and nanowires. To enhance the computational efficiency of MD, we proposed a novel atomic finite element method which has been proved to be much faster than the MD when the number of atoms is large. Obviously, the development of electromechanically coupled computational mechanics methods at multiscale is greatly beneficial not only to scientific research of material properties and electromechanical behavior such as deformation and fracture for piezoelectric/ferroelectric materials, but also to the structural design and reliability analysis of smart devices in engineering. It should be pointed out that all the computational methods presented in this lecture are only valid in their own scale because of the distinct fundamental assumptions in each method. Indeed, it is important to pass results from one scale to another in solving multi-scale problems. However, for general transfer of the material properties, it may be very difficult or impossible because the material properties at different scales are not comparable or not available at all. So far, a truly cross-scale computational method for ferroelectrics is still lacking which may hinder the understanding of ferroelectricity and piezoelectricity at multi-scale. Hence, hard work is needed in future to develop truly cross-scale computational methods.