Phase-field simulation of flexoelectricity in ferroelectrics by mixed finite element method

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ABSTRACT

Flexoelectricity describes the linear coupling between the electric polarization and the mechanical strain gradient or that between the mechanical strain and the polarization gradient. [1] Unlike other electromechanical coupling effects such as piezoelectricity and electrostriction, which require the non-centrosymmetric of the structure, flexoelectric effect appears in materials of any symmetry. Due to the low value of flexoelectric coefficients, the research on flexoelectricity in solids had long been overlooked, until a series of experimental observations about large flexoelectric effect of ferroelectric materials were reported by Ma and Cross in last decades. [2] The researchers are intrigued by these discoveries to study flexoelectricity and its applications, especially in nanoscale systems, which indicate bright prospect in utilizing flexoelectric effect of materials.

In this presentation, a continuum phase-field model of flexoelectricity is established in order to investigate the influence of flexoelectricity on the polarization and mechanical properties of ferroelectric materials. To deal with the high-order nature (strain gradient) originated from the flexoelectricity, a mixed finite element treatment is utilized. [3] For the ferroelectric properties, the polarization is regarded as the order parameter in phase field simulation. The evolution of the polarization is governed by the time-dependent Ginzburg-Landau equation. By 2-dimensional simulation, the comparison of the polarization between samples with and without flexoelectric effect is presented, which shows the importance of considering flexoelectric effect. Apart from that, the role of the boundary condition and the size effect are also studied. Some interesting phenomena, such as enhanced elasticity of cantilever induced by the coupling between strain gradient and polarization are revealed.

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