Pyroelectric and Dielectric Properties in Ferroelectrics with Bilayer and Compositionally-Graded Structures

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Ferroelectrics represent a group of functional materials with spontaneous polarization dependent of temperature, electric field, and strain. The pyroelectric and dielectric properties of ferroelectrics can be exploited for technological use in electronic devices, microsystems, computer memories, infrared detection, imaging, refrigeration, and power conversion. For these applications, ferroelectrics are usually integrated into thin film structures. Compared with bulk and homogeneous ferroelectric films, ferroelectric superlattices and compositionally-graded ferroelectrics show distinctive physical properties.

In this work, we focus on the ferroelectric/non-ferroelectric bilayer and compositionally-graded ferroelectric films. The computations are performed using nonlinear thermodynamic models based on Ginzburg-Landau-Devonshire theory by taking into account appropriate mechanical boundary conditions, and electrostrictive coupling of in-plane strains and polarization. In particular, we will take $BaTiO_3$ as the model ferroelectric layer in our studies on ferroelectric/non-ferroelectric bilayer. We will explore the phase diagram of the ferroelectrics under as a function of (1) in-plane misfit strain; (2) temperature; and (3) elastic properties, and (4) relative layer thickness of the non-ferroelectric layer. We will also take several scandate substrates as the model non-ferroelectric layer to discuss the roles of these four factors on polarization, pyroelectric coefficient and dielectric responses in $BaTiO_3$. Furthermore, we will describe the total free energy density in (001)-oriented, compositionally graded, and monodomain $Ba_{1-x}Sr_xTiO_3$ ferroelectric films including the relative contributions and importance of flexoelectric, gradient, and depolarization energy terms. We will discuss the effects of these energies on the evolution of the spontaneous polarization, the pyroelectric coefficient and dielectric permittivity as a function of position throughout the film thickness, temperature, and epitaxial strain. Overall, this work illustrates how temperature, strains, composition, and mechanical boundary conditions can be adjusted to deterministically control and engineer ferroelectrics with multilayer and compositionally-graded structures.