Thermodynamic Equilibrium of Strained Ferroelectric Thin Films and Heterostructures

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ABSTRACT

It has been well established that strains or stresses can have profound effects on the thermodynamic stability of phase and domain states of solids, and they can be judiciously utilized to tune solid state phase and domain microstructures and thus physical properties. In this presentation, I will discuss the mechanical equilibrium of strained ferroelectric thin films and heterostructures. In particular, I will show that one can efficiently construct incoherent multidomain and multiphase diagrams of arbitrarily strained or stressed ferroelectric thin films and heterostructures in analogy to the well-known temperature-composition phase diagrams. The corresponding coherent multidomain and multiphase diagrams, however, can only be established by computational methods, such as the phase-field method, by incorporating the coherency strain energy contributions as well as electrostatic interactions and domain wall energy contributions. One can also employ the phase-field method to predict the mesoscale topological transformations among the different ferroelectric polarization domain structures in the phase diagrams and possible presence of transient nonequilibrium mesoscale states. It will be shown that a combination of thermodynamic stability analysis and phase-field method offers a powerful theoretical tool for understanding the formation of thermodynamically stable, or the appearance of metastable/transient, mesoscale polar structures and for guiding the tuning of their properties.