FLAIR Colloquium

Thermodynamics of Ferroelectric Crystals with Domains

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The lecture discusses the thermodynamics and the phase-field method of ferroelectric crystals and their applications to modeling and predicting the stability of domain structures and their responses to mechanical and electric fields. It will start with the basic principles of classical thermodynamics by introducing a modern version of the first law of thermodynamics and apply it to obtain the fundamental equation of thermodynamics for homogeneous ferroelectric crystals. The relations of the fundamental equations of thermodynamics, Landau theory of ferroelectrics, and the thermodynamic properties will then be discussed, including the dielectric, elastic, piezoelectric properties. It will then be followed by the discussion on the thermodynamics of inhomogeneous ferroelectric crystals containing domain structures involving long-range elastic and electrostatic interactions and domain wall energy. The contributions to thermodynamics from electronic and ionic defects will be briefly discussed. The last part of the lecture will be focused on the applications of the phase-field method of ferroelectric domain structures. Examples will be presented to illustrate the application of the phase-field method to interpreting and understanding experimentally observed ferroelectric domain structures and to providing guidance to experimental growth of thin films and characterization to discover new mesoscale domain states of materials, achieve dramatically enhanced properties, and uncover hidden functionality.