A Non-Equilibrium Thermodynamics Framework for Domain Evolution; Phase Field Models and Finite Element Implementation

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Traditionally, the Ginzburg-Landau equation governing the evolution of domain configurations has been derived from a simple and physically justifiable set of assumptions. While this approach is certainly sound, it obscures the modern continuum physics distinction between fundamental balance laws, which are applicable to a wide range of materials, and the constitutive equations that are valid for a specific material. Here we present a small deformation non-equilibrium thermodynamics framework for ferroelectric domain evolution. In addition to the macro mechanical (static equilibrium) and electrical (Maxwell's laws) balance laws, we also postulate a micro-force balance governing a set of micro-forces forces (also called configurational forces) that are work conjugate to the order parameter, which in our case is the material polarization. Application of the second law of thermodynamics to this system allows us to identify general forms for the free energy and the dissipation coefficient of the material. The general form of the theory contains the standard Ginzburg-Landau equation as a special case. A finite element method for the solution of these types of phase field theories is described and implemented. Results from the model for domain wall structures and the pinning strength of an array of line charges will be presented.

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