

MAR11-2010-000914

Abstract for an Invited Paper  
for the MAR11 Meeting of  
the American Physical Society

### **Computational Design of Microstructures**

LONG-QING CHEN, Penn State University

Many important engineering materials are designed by controlling their phase transformations and microstructure evolution. Examples include the improvement of mechanical properties through solid state precipitation reactions in alloys such as Ni-based superalloys and age-hardened Al-alloys, the useful dielectric properties and electro-mechanical coupling effects by manipulating the phase transitions in ferroelectric crystals, the memory effect of shape-memory alloys by utilizing martensitic transformations. In this presentation, recent effort on integrating the phase-field approach with other computational methods such as first-principles calculations and CALPHAD will be discussed. A number of examples of coupling phase-field simulations and experimental measurements will be presented. It will be demonstrated that one can use the phase-field method to not only help interpreting experimental observations but also provide guidance to achieve desirable transition temperatures and specific domain/microstructure structures. The possibility to directly obtain the effective responses of a microstructure under an applied field from phase-field simulations, and thus the evolution of effective mechanical and transport properties will also be discussed.