MAR05-2005-020173

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Metastable Phase Evolution in Oxide Systems

CARLOS G. LEVI, Materials Department, University of California, Santa Barbara

Multi-component ceramics are often synthesized by routes that facilitate mixing at the molecular scale and subsequently generate a solid product at low homologous temperatures. Examples include chemical and physical vapor deposition, thermal spray, and pyrolytic decomposition of precursor solutions. In these processes the solid evolves rapidly from a highly energized state, typically in a temperature regime wherein long-range diffusion is largely constrained and the equilibrium configuration can be kinetically suppressed. The resulting product may exhibit various forms of metastability such as amorphization, nanocrystallinity, extended solid solubility and alternate crystalline forms. The approach allows access to novel combinations of structure and composition with unprecedented defect structures that, if reasonably durable, could have properties of potential technological interest. Understanding phase selection and evolution is facilitated by having a suitable reference framework depicting the thermodynamic hierarchy of the phases available to the system under the relevant processing conditions. When transformations are partitionless the phase menu and hierarchy can be readily derived from the relative position of the T0 curves/surfaces for the different pairs of phases. The result is a phase hierarchy map, which is an analog of the phase diagram for partitionless equilibrium. Such maps can then be used to assess the kinetic effects on the selection of metastable states and their subsequent evolution. This presentation will discuss the evolution of metastable phases in oxides, with emphasis on systems involving fluorite phases and their ordered or distorted derivatives. The concepts will be illustrated primarily with zirconia-based systems, notably those of interest in thermal barrier coatings, fuel cells and ferroelectrics (ZrO_2-$MO_{3/2}$, where M = Y, Sc, the lanthanides and combinations thereof, as well as ZrO_2-$YO_{3/2}$-TiO_2, ZrO_2-TiO_2-PbO, etc.). Of particular interest are the durabilities of metastable phases in systems that operate at high temperature, their decomposition paths and the implications to their functionality.