Novel Phase Diagram Behavior in Heterostructural Alloys

Scientific Achievement

We discovered wide metastable regions in the phase diagram of ***heterostructural*** alloys. The materials lie above the phase-separated free-energy minimum, but are stable against spinodal composition fluctuations.

Significance and Impact

Predictive synthesis of homogeneous single-phase alloys over a wide composition range will enable new Materials-by-Design strategies. The structural transition at the critical composition enables the ability to tune the properties in a non-linear or even discontinuous fashion.

Research Details

Theory: Density functional theory and the random phase approximation used to accurately calculate alloy phase diagrams.

Synthesis: (Mn,Zn)O by pulsed laser deposition and (Sn,Ca)S by RF sputtering using orthogonal composition and temperature gradients for both.

Characterization: Non-equilibrium phase diagrams and decomposition microstructures determined using XRD and STEM-EDS.

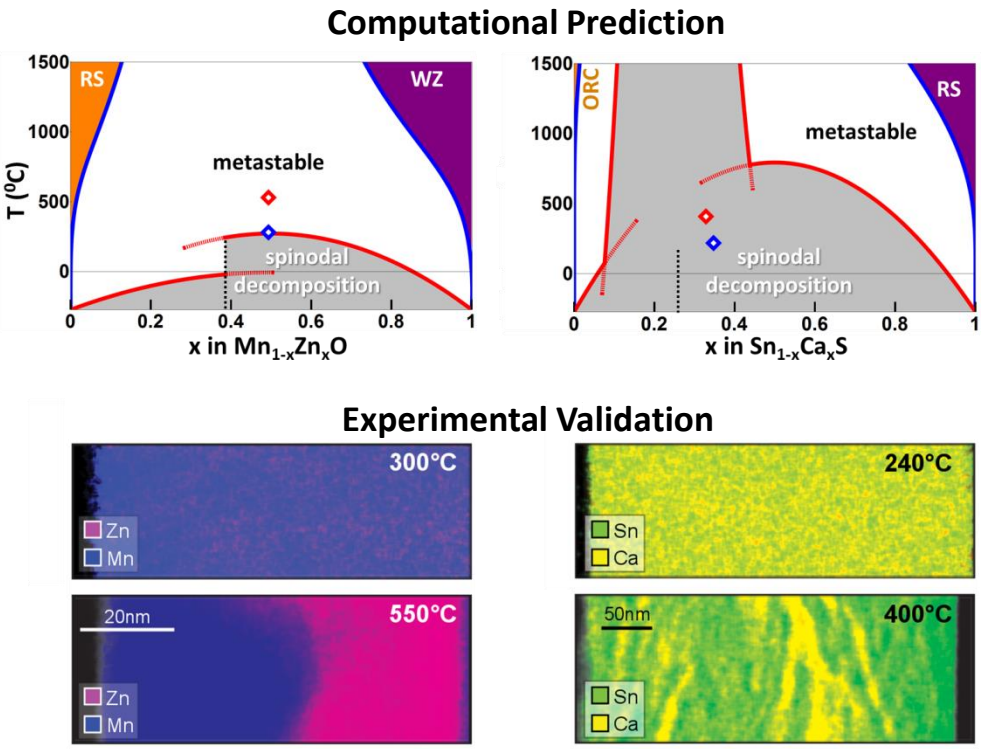

Figure: (Top) Predicted phase diagram of isostructural and heterostructural alloys. (Bottom) Spatial elemental composition maps for thin-film samples synthesized above and below the phase-separation temperature confirms the predicted binodal vs. spinodal decomposition mechanisms.

A.M. Holder, S. Siol, P.F. Ndione, H. Peng, A.M. Deml, B.E. Matthews, L.T. Schelhas, M.F. Toney, R.G. Gordon, W. Tumas, J.D. Perkins, D.S. Ginley, B.P. Gorman, J. Tate, A. Zakutayev, and S. Lany, *Science Advances*,**3** e1700270 (2017). DOI: 10.1126/sciadv.1700270

U.S. DEPARTMENT OF ENERGY | Office of Science | NREL NATIONAL RENEWABLE ENERGY LABORATORY | Massachusetts Institute of Technology | HARVARD UNIVERSITY | SLAC NATIONAL ACCELERATOR LABORATORY | OSU Oregon State University | MINES | BERKELEY LAB | CNGMD Incorporating Metastability