Thermodynamics of Roses-Toward Predictive Thermodynamic Models and Simulations

M. Stan[C, S], J.C. Ramirez, P. Cristea, M.I. Baskes, S.M. Valone and Z. Hu
Los Alamos National Laboratory, Los Alamos, NM, U.S.A.
mastan@lanl.gov

In one of his talks, Prof. Alan Oates presented a calculated ternary equilibrium phase diagram that looked much like a rose. He explained that he did that to demonstrate the versatility of the software and to show how, in principle, one can get any diagram they want. The implication was that some of the thermodynamic modeling work is purely descriptive, driven by prior knowledge of the target properties. This presentation reviews results, benefits, and challenges of making thermodynamics a less descriptive and more predictive science. It builds upon the work of Hume-Rothery and emphasizes the importance of turning electronic structure and atomistic calculations into trusted sources of information for thermodynamic models and simulations.

A new multi-scale and multi-physics method developed at LANL is presented. The method incorporates theory-based atomistic and continuum models into finite element simulations to predict thermo-mechanical properties of alloys and ceramics. By relating micro and nano-scale models to the macroscopic equilibrium and non-equilibrium simulations, the predictive character of the method is improved. The multi-scale approach is illustrated with recent results such as models pf phase stability in Pu-Ga alloys, calculations of defect concentration in CeO_{2-x} and PuO_{2-x}, and simulations of heat and mass transport in UO_{2-x}. The self-consistency of the approach is emphasized and potential sources of errors identified.