Model for Equation of State and Solidus and Liquidus of a Mixture for Description of High-Entropy Alloys

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Abstract

Self-consistent thermodynamic description of a mixture (a compound, an alloy, etc.) including both its equation of state (EOS) and solidus and liquidus surfaces (lines in the case of a binary mixture) is a challenging problem. We review several standard approaches with the associated mixing rules and discuss their shortcomings. We propose a new thermodynamics-based analytic model for the EOS of a N-component mixture, N ≥ 2. The model uses N−1 free parameters the values of which can be easily determined from the available experimental data on the binary subsystems; examples of such subsystems are shown in Figures 1 and 2. The knowledge of these parameters is required for the construction of the EOS. However, the calculation of both the solidus and liquidus surfaces of a N-component mixture, which the model also suggests, requires the knowledge of the melting curves of each of the constituents of the mixture, but no other information such as their EOSs is really needed. We apply the new model to multi-component mixtures of transition metals, emphasizing its suitability for the description of high-entropy alloys (HEAs), a revolutionary class of materials that depart from traditional metallurgy — which uses one base metal with minor additions — by mixing five or more elements in nearly equal proportions. An example of a quinary A-B-C-D-E HEA is shown in Figure 3. This approach creates a "high-entropy" effect that stabilizes simple solid-solution crystalline structures, resulting in materials with exceptional strength, fracture toughness, and resistance to corrosion and high temperatures. Our examples of the application of the new model to real multi-component systems will include both the ternary Cu-Pd-Pt alloy and ThO_2-UO_2-PuO_2 mixed-oxides (MOX) fuel system, the quaternary U-Pu-Nb-Zr alloy, and the quinary V-Nb-Ta-Mo-W HEA.

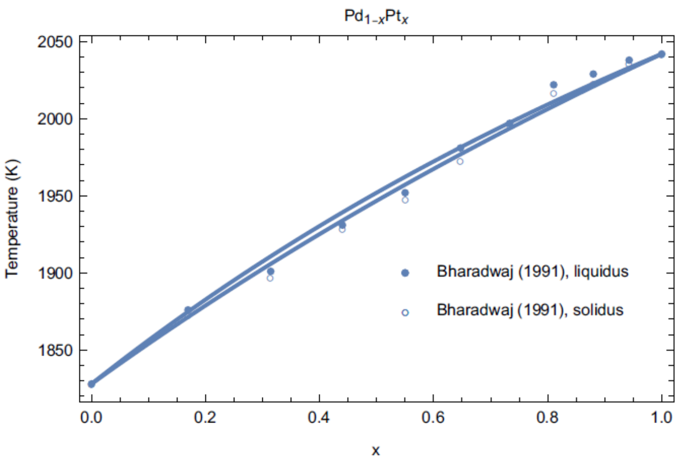

Figure 1. The high-T portion of the phase diagram of Pd-Pt system: Comparison of the new mixing model (lines) to the experimental data of Bharadwaj of 1991.

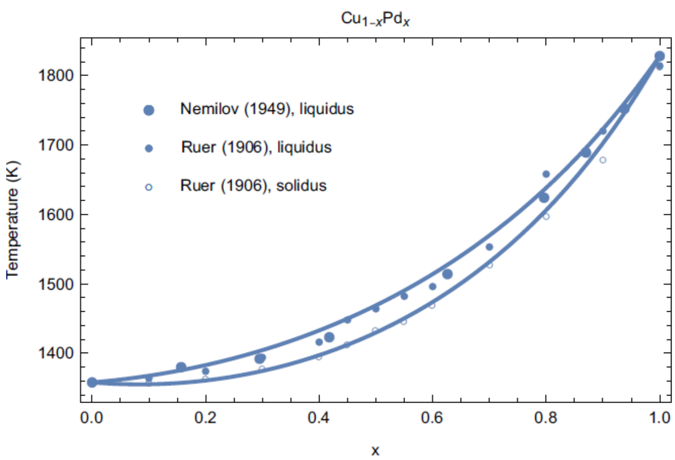

Figure 2. The high-T portion of the phase diagram of Cu-Pd system: Comparison of the new mixing model (lines) to the available experimental data from two sources.

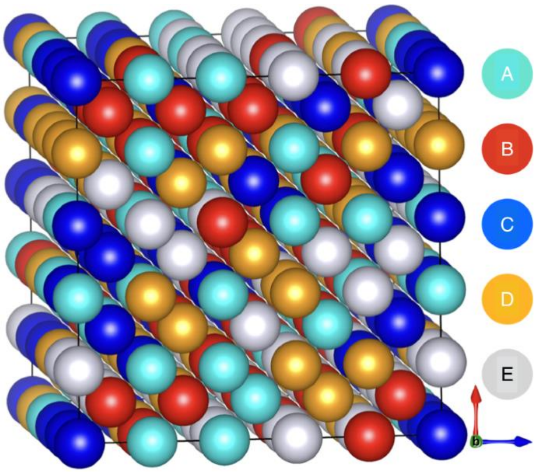

Figure 3. Example of HEA: a quinary A-B-C-D-E system; letters represent different transition metals.