Determining High-Pressure Binary Phase Diagram Evolution through Thermodynamics and Electrical Measurements

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Abstract

Understanding phase diagrams under high pressure is essential for predicting phase stability and transformations in materials. In this work, pressure-dependent phase diagrams of the Ga-based (Ga-Sn, Ga-In) and Bi-Pb binary systems were investigated using thermodynamic modeling and experimentally validated with electrical measurements in the Paris-Edinburgh press.

The phase diagrams were calculated using a pressure-dependent sub-regular solution model that incorporates the effect of pressure on Gibbs free energy and interaction parameters. The model also includes the effects of solid-phase transitions in the elements. The results demonstrate that pressure significantly modifies phase equilibria, shifting invariance temperatures and compositions, and altering liquidus curvature. A key finding is that pressure-induced solid-state phase transitions in the elemental constituents (Ga, Sn, Bi) strongly influence the topology of the phase diagrams. These transitions lead to the appearance or disappearance of phase regions, liquidus branching, and changes in phase stability fields. Across all systems, good agreement between calculated and experimental data confirms the reliability of the combined thermodynamic-experimental approach.

This study highlights the critical role of elemental phase transitions in shaping high-pressure phase diagrams and demonstrates the effectiveness of coupling thermodynamic modeling with high P-T electrical measurements to investigate phase behavior under extreme conditions.