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Theoretical Prediction of Activities in Dilute .γ-Ni(Al) Solid Solution at Elevated Temperatures YONG JIANG, JOHN SMITH, ANTHONY EVANS, UNIVERSITY OF CALIFORNIA, SANTA BARBARA, CA, USA COLLABORATION — For the prediction and interpretation of high-temperature diffusion and related phenomena in multiplayer systems, knowledge of thermodynamic activities is essential. For example, interfacial structures and adhesion strengths of .γ-Ni(Al)/Al2O3 at elevated temperatures strongly depend on Al activities. In this study, we present a method for predicting activity coefficients and hence activities in dilute .γ-Ni(Al) solid solutions from first-principles. Both thermal lattice vibration and electronic contributions to free energies are considered and compared. Vibrational contributions tend to dominate the temperature dependencies of the free energies: though electron thermal effects are significant. Calculations show opposing temperature trends for the formation enthalpies and entropies, leading to a partial cancellation of their role in the overall energetics. Nevertheless, their remaining temperature effects are strong. Over the temperature range, 400 K $<$ T $<$ 1700 K, the Al activity coefficient varies by 15 orders of magnitude, due to the relative strength of Al-Ni and Al-Al bonds. The Ni activity coefficient only varies less than 4% over the same range. Calculational results compare well with available experimental data. The thermodynamic principles elucidated from the calculations are used to provide a fundamental interpretation.

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