Combined Phase Diagram/Thermodynamic Properties Assessment of the Pt-Si and Th-Si Systems

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A major theme of Prof. Wayne Worrell's research during the 1960's and 1970's was the measurement of Gibbs energies of formation of highly stable intermetallic compounds in binary systems such as Pt-Ti, Pt-Zr, Pt-Hf, Pt-Al, and Pt-Ta (1-3). The high thermodynamic stabilities of such intermetallic compounds can lead to undesired high-temperature reactions. For instance, although platinum and SiO_2 are thermodynamically compatible in oxidizing atmospheres, in reducing atmospheres they can react to form Pt_xSi_y intermetallics according to

$$ySiO_2 + xPt = Pt_xSi_y + yO_2(g) \quad (1)$$

Similar reactions can occur in halide-containing systems, for instance

$$ySiI_4(g) + xPt = Pt_xSi_y + 4yI(g) \quad (2)$$

Formation of stable intermetallic compounds according to reactions similar to (1) and (2) causes undesirable effects such as degradation of Pt-containing thermocouples by formation of brittle intermetallic compounds. Another deleterious side effect is the release of reactive gases such as O_2 or I, which can cause undesirable reactions elsewhere in the system.

The understanding and control of reactions involving stable intermetallics requires measurement or estimation of their thermodynamic properties. Such measurements are incomplete or lacking in most binary intermetallic-forming systems. Combined assessment of phase diagram and thermodynamic properties data is a powerful method of generating estimates of thermodynamic properties of intermetallics which are internally consistent and consistent with the measured phase diagram. The use of phase diagram data for estimation of thermodynamic properties was pioneered, among others, by Erwin Rudy and Larry Kaufman, and was routinely taught by Prof. Worrell as early as the 1960's.

In this presentation, critical assessment techniques are used to generate optimized descriptions of thermodynamic properties of stable phases in the Pt-Si and Th-Si systems, using both the limited experimental thermodynamic data and phase diagram data. These systems contain 7 and 4 intermetallic compounds, respectively. The ASSESSMENT module of the thermodynamics software package MTDATA has been used to perform the optimization. Typical applications of the optimized thermodynamic parameters of the various phases are described.

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References

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