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Thermodynamic properties of the Pt-Fe system

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ABSTRACT

We determined activity-composition relationships for the Pt-Fe system by equilibrating Fe-oxides with Pt-Fe alloys at temperatures in the range of 1200–1400 °C and oxygen fugacities from 1.6 to 7.7 log units above the iron-wüstite (IW) buffer. The system is characterized by strong negative deviations from ideality throughout the investigated temperature range (e.g., $\gamma_{Fe}^{alloy}<0.02$ for $X_{Fe}^{alloy}<0.3$). Our data are consistent with an asymmetric regular solution of the form:

$$RT \ln \gamma_{Fe}^{alloy} = [W_{G_1} + 2(W_{G_2} - W_{G_1}) X_{Fe}^{alloy}](X_{Pt}^{alloy})^2$$

where $W_{G1} = -138.0 \pm 3.3$ kJ/mol and $W_{G2} = -90.8 \pm 24.0$ kJ/mol (1σ). Based on experiments at 1200–1400 °C, variations in the activity coefficients at a given composition are consistent with $\ln \gamma_{Fe}^{alloy}(T_1) / \ln \gamma_{Fe}^{alloy}(T_2) = T_2 / T_1$.

The Pt-Fe alloy composition in equilibrium with a FeO-bearing silicate liquid can be obtained from:

$$\log_{10} f_{O_2} = \log\{\exp[\ln a_{Fe_2SiO_4}^{liq} - \ln a_{SiO_2}^{liq} - 2\ln a_{Fe}^{alloy} - (\frac{-\Delta G_r^0}{RT})]\}$$

where ΔG_r^0 is the standard state free energy for the reaction $2Fe^{alloy} + O_2^{gas} + SiO_2^{liq} = Fe_2SiO_4^{liq}$. We obtained values of a_{Fe}^{alloy} from our model and used the program MELTS together with the thermodynamic properties of these elements to evaluate activities of SiO_2 and Fe_2SiO_4 components in the liquid and ΔG_r^0. We provide sample calculations showing how to predict the optimum Fe concentrations for pre-saturation of Pt-bearing containers to reduce Fe loss from the charge during experiments on magmatic liquids at high temperatures and pressures from 1 atm to 40 kbar.