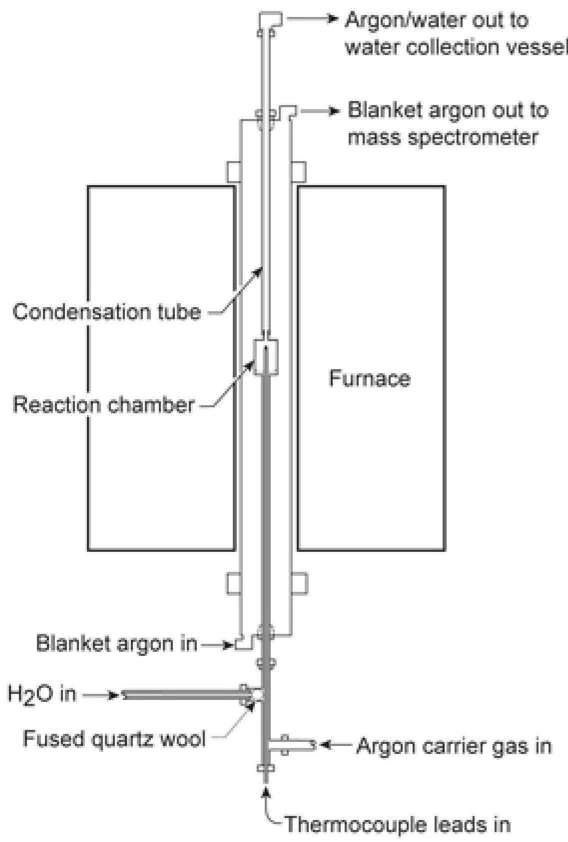
Thermodynamics of Volatile Species in the Silicon-Oxygen-Hydrogen System Studied

The volatilization of silica (SiO_2) to silicon hydroxides and oxyhydroxides because of reaction with water vapor is important in a variety of high-temperature corrosion processes. For example, the lifetimes of silicon carbide (SiC) and silicon nitride (Si_3N_4) -based components in combustion environments are limited by silica volatility. To understand and model this process, it is essential to have accurate thermodynamic data for the formation of volatile silicon hydroxides and oxyhydroxides.



Transpiration apparatus.

Long description of figure. Illustration showing thermocouple leads in, argon carrier gas in, fused quartz wool, water in, blanket argon in, reaction chamber, condensation tube, furnace, blanket argon out to mass spectrometer, and argon/water out to water collection vessel.

This reaction was studied at the NASA Glenn Research Center with a transpiration apparatus, illustrated in the preceding figure. A silica sample was reacted with gas streams containing controlled amounts of water vapor, and the resultant silicon-oxygen-hydrogen (Si-O-H) vapor species condensed downstream. From the amount of condensate, accurate vapor pressures could be determined. The vapor pressure as a function of pressure indicated that the following two reactions are likely:

$$SiO_2(s) + 2\ H_2O(g) = Si(OH)_4(g)$$

$$SiO_2(s) + H_2O(g) = SiO(OH)_2(g)$$

We found that the first reaction was significant over the whole temperature range studied (1073 to 1728 K), whereas the second reaction became important at the highest temperatures (1673 to 1728 K).

Temperature-dependent vapor pressure measurements lead to thermodynamic data. Second law measurements lead to a heat of formation $\Delta_f H°$ (1200) = –1354±2.7 kJ/mol and entropy $S°$ (1200) = 544.4±2.1 kJ/mol-K. Third law measurements lead to $\Delta_f H°$ (298) = –1344.3±1.2 kJ/mol. These are in very good agreement with previous measurements and previous ab initio calculations. A third law analysis of the high-temperature data led to a $\Delta_f H°$(298) for $SiO(OH)_2(g)$ of -831±5 kJ/mol. This value is also consistent with previous experiments.

Find out more about this research at http://www.grc.nasa.gov/WWW/EDB/

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