Equations of state and phase diagram of SiO_2 to lower mantle conditions

REBECCA A. FISCHER[1], ANDREW J. CAMPBELL[2], BETHANY A. CHIDESTER[3], DANIEL M. REAMAN[2], ELIZABETH C. THOMPSON[2], JEFFREY S. PIGOTT[4], VITALI B. PRAKAPENKA[5], AND JESSE S. SMITH[6]

[1] Harvard U., Dept. of Earth & Planetary Sci.
[2]U. Chicago, Dept. of the Geophysical Sci.
[3]U. California Davis, Dept. of Earth & Planetary Sci.
[4]Case Western Reserve U., Dept. of Earth, Env. & Planet. Sci.
[5]U. Chicago, Center for Advanced Radiation Sources
[6]High P. Collaborative Access Team, Carnegie Inst. Wash.

Silica is thought to be present in the Earth's lower mantle in subducting plates. It is known to undergo a phase transition from stishovite to the $CaCl_2$-type structure at ~50–80 GPa, but the exact location and slope of the phase boundary in pressure-temperature space is unresolved. There have been many previous studies on the equation of state of stishovite, but they span a limited range of pressures and temperatures, and there has been no thermal equation of state of $CaCl_2$-type SiO_2 measured under static conditions. We have investigated the phase diagram and equations of state of silica at 21–89 GPa and up to ~3300 K using synchrotron X-ray diffraction in a laser-heated diamond anvil cell. The phase boundary between stishovite and $CaCl_2$-type SiO_2 can be approximately described as $T = 64.6(49)*P - 2830(350)$, with temperature T in Kelvin and pressure P in GPa. The stishovite data imply $K_0' = 5.24(9)$ and a quasi-anharmonic T^2 dependence of $-6.0(4) \times 10^{-6}$ GPa*cm^3/mol/K^2 for a fixed $q = 1$, $\gamma_0 = 1.71$, and $K_0 = 302$ GPa, while for the $CaCl_2$-type phase $K_0 = 341(4)$ GPa, $K_0' = 3.20(16)$, and $\gamma_0 = 2.14(4)$ with other parameters equal to their values for stishovite. The behaviors of the *a* and *c* axes of stishovite with pressure and temperature were also fit, indicating a much more compressible *c* axis with a lower thermal expansion as compared to the *a* axis. The phase transition between stishovite and $CaCl_2$-type silica should occur at pressures of 68–78 GPa in the Earth, depending on the temperature in subducting slabs. Silica is denser than surrounding mantle material up to pressures of 58–68 GPa, with uncertainty due to temperature effects; at higher pressures than this, SiO_2 becomes gravitationally buoyant in the lower mantle.