

Equations of state and phase boundary for stishovite and CaCl₂-type SiO₂

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ABSTRACT

Silica is thought to be present in the Earth's lower mantle in subducting plates, in addition to being a prototypical solid whose physical properties are of broad interest. It is known to undergo a phase transition from stishovite to the CaCl₂-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 CaCl₂-type SiO₂ 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 CaCl₂-type SiO₂ can be approximately described as $T = 64.6(49) \cdot P - 2830(350)$, 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·cm³/mol/K² for a fixed $q = 1$, $\gamma_0 = 1.71$, and $K_0 = 302$ GPa, while for the CaCl₂-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 CaCl₂-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, SiO₂ becomes gravitationally buoyant in the lower mantle.

Keywords: Silica, SiO₂, stishovite, phase diagram, equation of state, phase transition, X-ray diffraction