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# High-pressure silica phase transitions: Implications for deep mantle dynamics and silica crystallization in the protocore

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## Abstract

The subsolidus phase diagram of silica in the 80–220 GPa pressure range was determined by density functional theory (DFT). The transition pressures calculated using the generalized gradient approximation (GGA) in the static limit (at 0 K, without zero point vibrational energy) for the β-stishovite ($CaCl_2$-structure) to seifertite and the seifertite to pyrite-type transitions are 95 and 213 GPa, respectively. These are in good agreement with those calculated using hybrid functionals, giving transition pressures of 96 and 215 GPa. This indicates that previous local density approximation (LDA) results underestimate the transition pressure by 10–15 GPa. Density functional perturbation theory calculations, carried out using GGA within the quasi-harmonic approximations, give Clapeyron slopes of 5.4 and –2.8 MPa/K for the β-stishovite to seifertite and seifertite to pyrite-type transitions, respectively. This suggests that the seifertite-forming transition occurs at 109 GPa (470 km above the core-mantle boundary, CMB) at an ambient mantle geotherm, whereas the pyrite-type transition occurs at 200 GPa (620 km below the CMB) at 4700 K, which is close to the core adiabat. We also calculate the equation of state and show that the stability of seifertite in the lowermost mantle contributes negative buoyancy to recycled oceanic crust, although not as much as in some previous studies. Nevertheless, the increased density of seifertite over β-stishovite may lead to layers with elevated proportions of basaltic material within the large low S-wave velocity provinces. The seifertite to pyrite-type silica transition in the outer core will affect the silica liquidus surface in the system Fe-Si-O and forms a basis for further investigations of silica crystallization in the protocore.

**Keywords:** Density functional theory, high-pressure silica polymorphs, deep mantle dynamics, silica crystallization in protocore, modified stishovite, seifertite, pyrite-type silica