

Stability of CaCl₂-type and alpha-PbO₂-type SiO₂ at high pressure and temperature determined by in-situ X-ray measurements

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SiO₂ is the most abundant oxide component in Earth's crust and mantle, and its high pressure phase transition has been of great interest. Previous experimental reports, however, have been controversial (e.g., Andraut et al. 1998; Dubrovinsky et al. 2001). To clarify the stable silica phase in the lower mantle, we conducted high pressure and temperature experiments in a laser-heated diamond anvil cell with in-situ X-ray diffraction measurements at the synchrotron facility SPring-8. Amorphous silica mixed with platinum powder was used as starting material. The sample was heated with a focused multimode Nd:YAG laser using double-sided heating technique. Angle-dispersive X-ray diffraction spectra were obtained by an imaging plate. We performed three runs at pressures between 101 and 151 GPa and temperatures between 2100 and 2500-K. To minimize kinetic effects, we compressed an amorphous sample to a high-pressure condition of interest and then heated in each experiment. The first run was conducted at 101-104 GPa and 2320-2450-K. After heating for 0.5 hr, the diffraction peaks of CaCl₂-type structure were clearly recognized, and did not change in the following heating for another 1 hr. The second run was performed at 124-128 GPa and 2250-2500-K. The diffraction lines of the α-PbO₂-type structure were clearly seen during heating for 2 hr. The third run was conducted at 113-117 GPa and 2160-2320-K. We observed diffraction peaks both of CaCl₂-type and α-PbO₂-type phase with similar intensities after the first 5 min heating. In the subsequent heating at 2200-2300-K, the CaCl₂-type silica became a dominant phase. We then compressed this sample to 130 GPa. During the sample was heated at 2100-2200 K, the relative intensities of the α-PbO₂-type structure were getting stronger with time. The results demonstrated that the CaCl₂-type silica is a post-stishovite phase and that it undergoes further transition to the α-PbO₂-type structure above 121 GPa at 2400-K. Present data together with previous first-principles calculations (Karki et al., 1997) indicate that the phase boundary between CaCl₂-type and α-PbO₂-type silica is represented by a linear equation $P \text{ (GPa)} = 98 + (0.0095 \pm 0.0016) * T \text{ (K)}$. This phase transition might contribute to the seismic wave velocity anomalies observed in the D double prime region.