



High-pressure behavior of cristobalite under quasi-hydrostatic conditions

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Cristobalite is a high-temperature, low-pressure polymorph of SiO_2 . It is comprised of a framework of SiO_4 tetrahedra, like many other low-pressure silica polymorphs, e.g. quartz tridymite, or coesite. Its cubic form known as β -cristobalite crystallizes above 1470 °C and at atmospheric pressure. The tetragonal α -phase is a metastable polymorph which appears upon cooling of the cubic β -cristobalite to ambient temperature and it can be found in natural acidic volcanic rocks.

High-pressure behavior of α -cristobalite is of interest from the geological standpoint because it was experimentally observed that under elevated pressures and at ambient temperature this polymorph with 4-fold coordinated silicon can transform to *seifertite* – a lower mantle phase with octahedrally coordinated Si. The transformational sequence is as follows. The tetragonal α -cristobalite transforms to a monoclinic cristobalite II near ~ 1.5 GPa upon hydrostatic compression. The structure of this higher-pressure polymorph was recently solved. Above ~ 10 GPa cristobalite II is found to transform to cristobalite X-I. Apart from the recent determination of the unit cell parameters, the structure of the cristobalite X-I still remains unknown. Further compression of cristobalite X-I above pressures exceeding ~ 35 GPa leads to formation of cristobalite X-II, which is the polymorph reported to have the structure of seifertite. However, there is a large discrepancy among various experimental observations regarding the pressure at which this transition takes place. Motivated by the recent studies, we aim at understanding how the structure of this "bridging phase", cristobalite X-I, is evolving under pressure and how it transforms to the seifertite phase.

We performed in-situ single crystal Raman spectroscopy and X-ray diffraction up to 82 GPa in steps of 3-5 GPa. We used diamond-anvil cells with 250 μm diamond culet size and neon as the pressure-transmitting medium. In-situ Raman spectra indicated the phase transition to cristobalite II near 1.5 GPa and the formation of the X-I phase above 10 GPa, in agreement with previous studies. This high-pressure phase persists up the highest pressures achieved and it is not quenchable – upon decompression it retransforms into a phase with Raman spectra very similar to that of the starting α -cristobalite. Single crystal X-ray diffraction data were collected at Extreme Conditions Beamline P02.2 at Petra III. We confirmed the phase transition to cristobalite II and further above 10 GPa to the phase X-I. Indexing of the diffraction patterns of the phase X-I collected at 17 GPa yields a primitive monoclinic unit cell with $a = 6.5899(9)$ Å, $b = 4.0493(6)$ Å, $c = 6.841(8)$ Å, $\beta = 98.15(3)^\circ$ and the most likely space groups $P2_1/c$ or $P2_1/n$. A preliminary structure analysis reveals that all Si atoms are octahedrally coordinated at this pressure. Single-crystal X-ray diffraction data from experiments at higher pressures are currently being analyzed.