The behavior of single-crystal cristobalite X-I under dynamic decompression

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Found in a variety of geological environments, SiO_2 exhibits complex phase behavior upon changes in pressure and temperature. The variety of phase transitions exhibited by silica can be attributed to its exceptionally strong Si-O bond, and silicon's ability to shift between fourfold and sixfold coordination with pressure [1, 2]. In between stable high temperature and high pressure polymorphs, a number of metastable phases exist, which are of great interest in understanding dynamic structural phenomena [3, 4].

For cristobalite, a high-temperature polymorph of SiO_2, a complex system of pressure-dependent phase transitions has been previously reported. Starting with α-cristobalite, a reversible change to the monoclinic cristobalite-II takes place at 1.8 GPa [5], and was observed to be suppressed up to 10 GPa with a sufficiently rapid increase in pressure [6]. An additional, non-quenchable change to cristobalite X-I was observed at approximately 12 GPa, which persists until at least 80 GPa [1, 4]. There is little consensus on the stability and structure of this X-I phase, despite repeated experimental efforts; recent publications have shown a structure with octahedrally coordinated silicon, despite relatively low pressures and ambient temperature [4]. This unusual phase may be a structural bridge between low-pressure tetrahedrally coordinated and high-pressure octahedrally coordinated phases of SiO_2.

In contrast to other studies documenting cristobalite X-I past its formation pressure, we observed this phase's decompression behavior in a dynamic environment within a membrane-driven diamond anvil cell. Starting at 12.5 GPa, we observed the existence of cristobalite X-I to approximately 4.7 GPa, and were able to elaborate on existing equations of state. At this pressure, cristobalite X-I is well outside its previously determined stability field, and into the territory at which cristobalite-II should be seen. The persistence of this phase with decompression, along with the previous rate-dependent suppression of phase transitions, implies that the rate of pressurization is crucial in understanding the formation of high-pressure SiO_2 phases.

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