American Mineralogist, Volume 99, pages 184–189, 2014

Crystal structures and stabilities of cristobalite-helium phases at high pressures

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Abstract

First-principles calculations were used to study the structural and energetic properties of cristobalite-He I and II at high pressures, both of which were recently found in high-pressure powder X-ray diffraction experiments of α-cristobalite with helium pressure-medium at room temperature. These calculations have revealed that both cristobalite-He I and II contain one helium atom per SiO_2 with the formula SiO_2He. It has also been revealed that cristobalite-He I is energetically favored above 6.4 GPa, cristobalite-He II is the stable phase at pressures between 1.7 and 6.4 GPa, and the mixture of cristobalite II and crystalline He is more stable than either cristobalite-He I or II below 1.7 GPa, in general agreement with the observation. Cristobalite-He I and II have been predicted to be monoclinic with space group $P2_1/c$, and rhombohedral with space group $R\bar{3}c$, respectively. The unit-cell parameters of both cristobalite-He I and II were re-determined from the previously measured high-pressure X-ray diffraction data on the basis of these predicted cells. There is an excellent agreement between the observed (re-determined) and calculated pressure dependence of the cell parameters for the both phases. The calculated X-ray diffraction patterns for both cristobalite-He I and II are also consistent with the observed data. Cristobalite-He I and II have been predicted to have molar volumes 21% larger at 10 GPa and 23% larger at 4 GPa than cristobalite II due to the penetration of helium atoms into large voids of the structure.

Keywords: Cristobalite-helium, high pressure, stability, first-principles calculations