

Crystal structure of CaSiO₃ perovskite at 28–62 GPa and 300 K under quasi-hydrostatic stress conditions

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ABSTRACT

To find the thermodynamically stable crystal structure of CaSiO₃ perovskite (CaPv) at high pressure and 300 K, we have conducted synchrotron X-ray diffraction (XRD) on thermally stress-annealed samples in a Ne pressure medium in the diamond-anvil cell at 28–62 GPa. Rietveld refinements of the diffraction patterns are significantly improved in fitting the positions and intensities of the split lines of CaPv if the starting model is a tetragonal perovskite-type structure with the SiO₆ octahedral rotation around the tetragonal *c*-axis. The result is in contrast with other previous experiments, but is consistent with first-principles calculations, reconciling the discrepancy between computations and experiments on the crystal structure of CaPv. We attribute the observed difference to the formation of the thermodynamically more stable phase under improved stress conditions in our experiments. Our fitting shows that the bulk modulus of CaPv is 223 ± 6 GPa when its pressure derivative fixed to 4, which is also consistent with first-principles calculations. The previous observations of the diffraction patterns of CaPv inconsistent with the first-principles studies could be due to the formation of a metastable crystal structure of CaPv under elevated deviatoric stresses.

Keywords: CaSiO₃ perovskite, crystal structure, hydrostatic stress, X-ray diffraction, equation of state