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High-pressure experimental study of tetragonal $CaSiO_3$-perovskite to 200 GPa

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Abstract

In this study, we have investigated the crystal structure and equation of state of tetragonal $CaSiO_3$-perovskite up to 200 GPa using synchrotron X-ray diffraction in laser-heated diamond-anvil cells. X-ray diffraction patterns of the quenched $CaSiO_3$-perovskite above 148 GPa clearly show that 200, 211, and 220 peaks of the cubic phase split into 004+220, 204+312, and 224+400 peak pairs, respectively, in the tetragonal structure, and their calculated full-width at half maximum (FWHM) exhibits a substantial increase with pressure. The distribution of diffraction peaks suggests that the tetragonal $CaSiO_3$-perovskite most likely has an *I*4/*mcm* space group at 300 K between 148 and 199 GPa, although other possibilities might still exist. Using the Birch-Murnaghan equations, we have determined the equation of state of tetragonal $CaSiO_3$-perovskite, yielding the bulk modulus $K_{0T} = 227(21)$ GPa with the pressure derivative of the bulk modulus, $K'_{0T} = 4.0(3)$. Modeled sound velocities at 580 K and around 50 GPa using our results and literature values show the difference in the compressional (V_P) and shear-wave velocity (V_S) between the tetragonal and cubic phases to be 5.3 and 6.7%, respectively. At ~110 GPa and 1000 K, this phase transition leads to a 4.3 and 9.1% jump in V_P and V_S, respectively. Since the addition of Ti can elevate the transition temperature, the transition from the tetragonal to cubic phase may have a seismic signature compatible with the observed mid-lower mantle discontinuity around the cold subduction slabs, which needs to be explored in future studies.

Keywords: Tetragonal $CaSiO_3$-perovskite, equation of state, crystal structure, high pressure