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Cubic perovskite polymorph of strontium metasilicate at high pressures

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Abstract

By using a diamond-anvil cell (DAC) with laser heating technology, a cubic perovskite polymorph of $SrSiO_3$ has been synthesized at ~38 GPa and 1500–2000 K for the first time. The *P-V* data of this new phase give ambient temperate elastic constants of $V_0 = 49.18(5)$ Å^3, $K_0 = 211(3)$ GPa, respectively, when they are fitted against the Birch-Murnaghan equation of state with a fixed K_0' at 4. On decompression, the $SrSiO_3$ cubic perovskite phase becomes unstable at ~6.2 GPa and disappears completely at ~4.7 GPa. The transformed product can be considered as an amorphous phase with a minor amount of small sized crystals in the amorphous matrix. First principle calculations predicted structural properties of both the cubic and the six-layer-repeated hexagonal perovskite polymorphs of $SrSiO_3$ in good agreement with experimental results. The experimental and theoretical results indicate that the larger Sr^{2+} cation can substitute the Ca^{2+} cation and enter into the lattice of the cubic perovskite phase of $CaSiO_3$ at lower mantle conditions with only a small lattice strain. These results indicate that Sr can be hosted in cubic perovskite $CaSiO_3$ found as inclusions in diamonds originating from the lower mantle.

Keywords: $SrSiO_3$, cubic perovskite, high pressure, equation of state