Thermal equation of state of post-aragonite $CaCO_3$ up to 85 GPa and 2500 K

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Subduction of carbonates is the main mechanism for transporting carbon from Earth's surface to the deep interior [1]. One of the most abundant carbonates and a potential major host for oxidized carbon in the deep Earth is $CaCO_3$. The stable polymorph of $CaCO_3$ in most of Earth's lower mantle (pressures ~45 GPa to ~130 GPa) has been predicted and observed to be the *Pmmn* post-aragonite structure [2-4], but the physical properties of this phase under lower mantle conditions are still uncertain. Understanding compressibility and thermal expansion of post-aragonite $CaCO_3$ at high-pressures and temperatures (H-*P*/*T*) will help constrain the role of the lower mantle in the deep carbon cycle. We examined post-aragonite $CaCO_3$ in the laser-heated diamond anvil cell at pressures ~47-88 GPa and temperatures up to 2500 K using synchrotron H-*P*/*T* X-ray diffraction at beamline 13-ID-D of the Advanced Photon Source. Post-aragonite $CaCO_3$ was synthesized from pure calcite powder by laser heating for 10 minutes at 1800 K and ~47 GPa. Complete transformation to the post-aragonite structure was confirmed by full-profile LeBail fitting. The ambient pressure unit-cell volume (V_0), bulk modulus (K_0) and its first derivative (K_0') were determined by fitting the third-order Birch-Murnaghan equation of state (BM-EOS) to our 300 K data, and the thermal expansion coefficient (α_T) and temperature derivative of the bulk modulus ($(\partial K_T/\partial T)_{0P}$) were obtained from a high-temperature BM-EOS fit to our high-temperature data. Using this *P*-*V*-*T* equation of state for post-aragonite $CaCO_3$ along the lower mantle geotherm (corresponding to ~ 45 - ~130 GPa and ~2200 - ~2800 K) [5], we calculated 14% and 8% lower density (ρ) relative to the Preliminary Reference Earth Model (PREM) at 45 and 130 GPa, respectively[6], indicating a smaller density contrast with increasing depth in the lower mantle. If $CaCO_3$ can be subducted into the lower mantle, the density increase due to the post-aragonite transition and high compressibility relative to silicates will promote the transport of $CaCO_3$ to core-mantle-boundary depth.

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