Experimental and theoretical thermal equations of state of $MgSiO_3$ post-perovskite at multi-megabar pressures

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The $MgSiO_3$ post-perovskite phase is the most abundant silicate phase in a super-Earth’s mantle, although it only exists within the Earth’s lowermost mantle. We established the thermal equations of state (EoS) of the $MgSiO_3$ post-perovskite phase, which were determined by using both laser-heated diamond anvil cell (LHDAC) and density-functional theoretical techniques, within a multi-megabar pressure range, corresponding to the conditions of a super-Earth’s mantle. The LHDAC experiments were performed at up to a pressure of 265 GPa at a temperature of 300 K, and 170 GPa at 2560 K. The *ab initio* calculations were performed at up to 1.2 TPa and 5000 K. The Keane and AP2 EoS models, which include parameters that limit to infinity at high pressure, were adopted for the first time to extract meaningful physical properties. The experimental volume data in a wide pressure-temperature range enabled us to determine the fully experimentally based parameters for the Mie-Grüneisen-Debye model. The Grüneisen parameter and its volume dependency were found to be consistent with their theoretically obtained values. Both the experimental and theoretical EoS are also found to be in very good agreement with one another, within 0.1% in volume at the earth’s core-mantle boundary condition, and the relation is maintained within 0.8% even up to a pressure and temperature of 300 GPa and 5000 K, respectively. Our newly developed EoS should be applicable to a super-Earth’s mantle, as well as the Earth’s core-mantle boundary region.

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