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Thermal equation of state and spin transition of magnesiosiderite at high pressure and temperature

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Abstract

In situ synchrotron X-ray diffraction experiments on natural magnesiosiderite [$(Mg_{0.35}Fe_{0.65})CO_3$] were conducted using resistive and laser-heated diamond-anvil cells (DACs) up to 78 GPa and 1200 K. Based on thermal elastic modeling of the measured pressure-volume curves at given temperatures, we have derived thermal equation of state (EoS) parameters and the spin-crossover diagram of magnesiosiderite across the spin transition. These results show the spin crossover broadened and shifted toward higher pressures at elevated temperatures. Low-spin magnesiosiderite is 6% denser and 8% more incompressible than the high-spin phase at 1200 K and high pressures. Within the spin crossover from 53 to 63 GPa at 1200 K, magnesiosiderite exhibits anomalous thermal elastic behaviors, including a dramatic increase in the thermal expansion coefficient by a factor of 20 and a drop in the isothermal bulk modulus and the bulk sound velocity by approximately 75 and 50%, respectively. Compared with the end-member magnesite [$MgCO_3$] at relevant pressure-temperature conditions of the subducted slabs, the high-spin magnesiosiderite with 65 mol% $FeCO_3$ is approximately 21–23% denser and its unit-cell volume is 2–4% larger, whereas the low-spin state is 28–29% denser and 2% smaller than the end-member magnesite. Since ferromagnesite with 20 mol% of iron has been proposed to be a potential deep-carbon carrier, our results here indicate that the dense low-spin ferromagnesite can become more stable than high-spin ferromagnesite at pressures above approximately 50 GPa, providing a mechanism for (MgFe)-bearing carbonate to be a major carbon host in the deeper lower mantle.

Keywords: Fe-rich carbonate, thermal equation of state, spin transition, ferromagnesite, diamond-anvil cell