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Thermoelastic parameters of Mg-sursassite and its relevance as a water carrier in subducting slabs

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Abstract

We report the synthesis, at 7 GPa and 923 K, and the thermoelastic characterization, up to 16 GPa and 850 K, of a single crystal of Mg-sursassite, $Mg_5Al_5Si_6O_{21}(OH)_7$. In situ high-pressure and high-temperature single-crystal diffraction allowed the study of structural variation at non-ambient conditions and the determination of bulk elastic properties. The refined parameters of a second-order Birch-Murnaghan equation of state (BM-II EoS) are $V_0 = 446.02(1)$ Å^3 and $K_{T0} = 135.6(7)$ GPa. The thermal expansion coefficients of a Berman-type EoS are $\alpha_0 = 3.14\ (5) \times 10^{-5}\ K^{-1}$, $\alpha_1 = 2.50(16) \times 10^{-8}\ K^{-2}$, and $V_0 = 445.94(3)$. For comparison, the *P-V* EoS is determined for a natural sursassite sample, ideally $Mn_4Al_6Si_6O_{22}(OH)_6$. The refined parameters of BM-II EoS [$V_0 = 470.2(3)$ Å^3, $K_{T0} = 128(4)$ GPa] indicate that composition has a minimal effect on elastic properties. The similarity of density and bulk properties of Mg-sursassite if compared to olivine and other anhydrous mantle minerals suggests that this phase could be overseen by geophysical methods.

Keywords: Mg-sursassite, hydrous minerals, crystal structure, thermoelastic parameters