P-V-T relations of γ-Ca₃(PO₄)₂ tuite determined by in situ X-ray diffraction in a large-volume high-pressure apparatus

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ABSTRACT

Tuite, γ -Ca₃(PO₄)₂, is regarded as an important phosphate mineral in the deep mantle playing a crucial role as a host for rare earth elements, large ion lithophile elements, and phosphorus. In this study we report the thermoelastic properties of synthetic γ -Ca₃(PO₄)₂ at simultaneously high pressures and temperatures of up to 35.4 GPa and 1300 K, respectively, as determined by means of in situ energy-dispersive X-ray diffraction in a large-volume multi-anvil apparatus. The pressure-volume-temperature data obtained for γ -Ca₃(PO₄)₂ were fitted by the high-temperature Birch-Murnaghan equation of state to yield $V_0 = 447.4(4)$ Å³, $K_{T0} = 100.8(18)$ GPa, $K'_{T0} = 5.74(13)$, ($\partial K_T/\partial T$)_P = -0.020(1) GPa/K, and $\alpha_T = 3.26(18) \times 10^{-5} + 1.76(24) \times 10^{-8} T$. In addition, fitting the present data to the Mie-Grüneisen-Debye equation of state gives $\gamma_0 = 1.35(6)$, $\Theta_0 = 944(136)$ K, and q = 0.37(29). Based on the thermoelastic properties obtained in our study, the density profiles of γ -Ca₃(PO₄)₂ tuite along typical cold and hot slab geotherms were calculated and are compared with those of the coexisting silicate minerals in subducting mid-ocean ridge basalt.

Keywords: γ -Ca₃(PO₄)₂ tuite, in situ X-ray diffraction, thermal equation of state, thermoelastic properties