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Thermal elastic behavior of $CaSiO_3$-walstromite: A powder X-ray diffraction study up to 900 °C

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Abstract

Walstromite-structured $CaSiO_3$ (Wal) was synthesized at 6 GPa and 1200 °C for 6 h using a cubic press, and its thermal elastic behavior was investigated at T up to 900 °C using a powder X-ray diffraction technique at ambient pressure. Within the investigated T range, all unit-cell parameters, j, of Wal varied almost linearly with T, so that we fitted the data with the equation $\alpha_j = j^{-1}(\partial j/\partial T)$ and obtained $\alpha_a = 0.92(2) \times 10^{-5}$/°C, $\alpha_b = 1.65(1) \times 10^{-5}$/°C, $\alpha_c = 0.83(1) \times 10^{-5}$/°C, and $\alpha_V = 3.24(3) \times 10^{-5}$/°C for Wal. The magnitudes of the principal Lagrangian strain coefficients (ε_1, ε_2, and ε_3) and the orientation of the thermal strain ellipsoids, between ambient T and measured T, were calculated. The orientation of the strain ellipsoid appears constant with T variation, whereas the strain magnitudes vary significantly with T: ε_1 increases, but ε_2 and ε_3 decrease. For $T > 900$ °C, primitive data were collected for "parawollastonite" (Wo-2*M*), which led to a much smaller volumetric thermal expansion coefficient than that of Wal.

Keywords: $CaSiO_3$-walstromite, high-P synthesizing, high-T X-ray diffraction, "parawollastonite", thermal elasticity