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, $a_i$, of Wal varied almost linearly with T, so that we fitted the data with the equation $a_i = j_i(\partial a_i/\partial T)$ and obtained $a_0 = 0.92(2) \times 10^{-5}/°C$, $a_1 = 1.65(1) \times 10^{-5}/°C$, $a_2 = 0.83(1) \times 10^{-5}/°C$, and $a_3 = 3.24(3) \times 10^{-5}/°C$ for Wal. The magnitudes of the principal Lagrangian strain coefficients ($\varepsilon_1$, $\varepsilon_2$, and $\varepsilon_3$) 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: $\varepsilon_1$ increases, but $\varepsilon_2$ and $\varepsilon_3$ decrease. For $T > 900 °C$, primitive data were collected for “parawollastonite” (Wo-2M), 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

INTRODUCTION

It has been well accepted by the scientific community that the mantle of the Earth is mainly peridotitic (pyrolite; Ringwood 1975), with some minor portions being eclogitic due to the recycling of the oceanic crust back to the deep interior of the Earth via the subduction process (Ringwood 1994; Hirose et al. 1999). Recently, many Ca-silicate phases such as walstromite-structured CaSiO$_3$ (Wal), titanite-structured CaSi$_2$O$_6$ (Ttn), and larnite ($\beta$-Ca$_3$SiO$_4$; Lrn) were discovered as inclusions in diamonds that probably originated from the lower mantle (Joswig et al. 1999; Jambor et al. 2000; Stachel et al. 2000; Nasdala et al. 2003; Brenker et al. 2005), indicating a potential Ca-rich lithology in the Earth’s deep mantle. Trace element analyses of these Ca-rich inclusions suggested extreme degrees of LREE (200–2000 times chondritic) and Sr enrichment (70–1000 times chondritic) together with negative and positive Eu anomalies (Stachel et al. 2000), suggesting that this Ca-rich lithology might be an important reservoir with distinctive geochemical features. For a better understanding of the physical-chemical interaction among these different lithologies in the deep interior of the Earth, it is apparently very important to study these Ca-rich phases.

To understand the geodynamic process that these natural Ca-rich inclusions in diamonds once experienced, the phase relationships in the composition CaSiO$_3$ at high P-T conditions are critical; these are well understood: Wal, Ttn, and Lrn are related by the reaction 3Wal = Ttn + Lrn, which takes place at about 8 GPa (Kanzaki et al. 1991; Wang and Weidner 1994; Gasparik et al. 1994; Kubo et al. 1997; Akaogi et al. 2004; Sueda et al. 2006). At a lower pressure of about 3 GPa (Essene 1974; Huang and Wyllie 1975; Chatterjee et al. 1984; Akaogi et al. 2004), Wal transforms to wollastonite-I (Wo; CaSiO$_3$; Barkley et al. 2011). At a higher pressure of about 12 GPa, Ttn and Lrn combine to form CaSiO$_3$-perovskite, the dominant Ca-bearing phase in the lower mantle of the Earth (Mao et al. 1977; Irifune et al. 1989; Tamai and Yagi 1989). To appreciate the incorporation of the trace elements, such as LREE and Sr, in these Ca-rich phases, on the other hand, detailed crystallographic and thermal elastic data are required (Blundy and Wood 1994; Law et al. 2000). As outlined by Swamy and Dubrovinsky (1997a) and Akaogi et al. (2004), however, many thermal elastic properties of Wal, Ttn, and Lrn have not been experimentally determined so far.

Wal (CaSiO$_3$; $P^1$) was first synthesized by Ringwood and Major (1967), with its first structure determination by Trojer [1969; $a = 6.695(5)$ Å, $b = 9.257(7)$ Å, $c = 6.666(6)$ Å, $\beta = 86°38′$, $\gamma = 76°08′$]. Joswig et al. (2003) detailed the crystal structure of Wal entrapped as inclusion in diamond by single-crystal X-ray diffraction, and also predicted its compression behavior up to about 35 GPa using density functional theory. Here we have investigated the thermal elasticity of Wal by powder X-ray diffraction at T up to ~900 °C.

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