P-V-T equation of state of Ca$_3$Cr$_2$Si$_3$O$_{12}$ uvarovite garnet by using a diamond-anvil cell and in-situ synchrotron X-ray diffraction

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ABSTRACT

The pressure-volume-temperature (P-V-T) equation of state (EoS) of synthetic uvarovite has been measured at high temperatures up to 900 K and high pressures up to 16.20 GPa, by using in situ angle-dispersive X-ray diffraction and diamond-anvil cell. Analysis of room-temperature P-V data to a third-order Birch-Murnaghan EoS yielded: $V_0 = 1736.9 \pm 0.5$ Å$^3$, $K_0 = 162 \pm 2$ GPa, and $K''_0 = 4.5 \pm 0.3$. With $K''_0$ fixed to 4.0, we obtained: $V_0 = 1736.5 \pm 0.3$ Å$^3$ and $K_0 = 164 \pm 1$ GPa. Fitting of our P-V-T data by means of the high-temperature third-order Birch-Murnaghan equations of state, given the thermoelastic parameters: $V_0 = 1736.8 \pm 0.8$ Å$^3$, $K_0 = 162 \pm 3$ GPa, $K''_0 = 4.3 \pm 0.4$, $(\partial K/\partial T)_p = -0.021 \pm 0.004$ GPa/K, and $\alpha_0 = (2.72 \pm 0.14) \times 10^{-5}$ K$^{-1}$. We compared our elastic parameters to the results from the previous studies for uvarovite. From the comparison of these fittings, we propose to constrain the bulk modulus and its pressure derivative to $K_0 = 162$ GPa and $K''_0 = 4.0 - 4.5$ for uvarovite. Present results were also compared with previous studies for other garnetite garnets, grossular and andradite, which indicated that the compression mechanism of uvarovite might be similar with grossular and andradite. Furthermore, a systematic relationship, $K_0$(GPa) = 398.1(7) - 0.136(8) $V_0$(Å$^3$) with a correlation coefficient $R^2$ of 0.9999, has been established based on these isostroanalogus. Combining these results with previous studies for pyralspite garnets—pyrope, almandine, and spessartine—the compositional dependence of the thermoelastic parameters (bulk modulus, thermal expansion, and the temperature derivative of the bulk modulus) were discussed.

Keywords: Uvarovite, equation of state, high pressure and high temperature, X-ray diffraction, diamond-anvil cell

INTRODUCTION

Silicate garnets are considered important rock-forming minerals of the Earth’s interior existing in the upper mantle and transition zone, comprising up to 40% by volume of the pyrolite composition and up to 70% of eclogite composition (Akaogi and Akimoto 1977; Anderson and Bass 1984; Irfune and Ringwood 1987; Ita and Stixrude 1992; Dymshits et al. 2014). They occur as stable phases in a wide range of pressures, temperatures, and chemical environments, and play a fundamental role in high-pressure and high-temperature petrogenetic processes (Deer et al. 1992; Pavese et al. 2001). Garnets are also important components of subducted oceanic crust, and it is suggested that garnet-rich subducted crust can be gravitationally trapped in the lowermost part of transition zone (Irfune and Ringwood 1993; Karato et al. 1995). In addition, former experiments at high pressure and high temperature on garnets showed that post-garnet transitions occur at pressure and temperature conditions relatively close to the ones of the 660 km depth discontinuity (Irfune et al. 1996; Akaogi et al. 1998; Gréaux et al. 2011a, 2011b). Therefore, understanding the thermoelastic properties of garnets is essential to infer appropriate compositional models and regional seismic profiles of the Earth’s interior (Duffy and Anderson 1989; Weidner and Wang 2000).

The mineral of the garnet group are divided into two series, pyralspite and ugrandite. Uvarovite is a chromium-bearing ugrandite garnet group species with the formula Ca$_3$Cr$_2$Si$_3$O$_{12}$ and is thus distinguished from both grossularite (Ca$_3$Al$_2$Si$_3$O$_{12}$) and andradite (Ca$_3$Fe$_2$Si$_3$O$_{12}$). Uvarovite is one of the rarest of the garnet group minerals, but nonetheless prevalent in many terrains and geologic settings (Green and Falloon 1998; O’Neill and Palme 1998; Chopelas 2005; Klemme et al. 2005), and its thermoelastic behavior at high pressure and high temperature will shed light on other ugrandite garnets, as well as pyralspite garnets. It can form a complete solid-solution series with grossular and andradite in the Earth’s interior (Huckenholz and Knittel 1975). Uvarovite has generally been found associated with serpentineite, chromite, metamorphic limestones, and skarn ore-bodies; it has formed from contact metamorphic processes or hydrothermal processes (Challis et al. 1995; Graham et al. 1996; Proenza et