American Mineralogist, Volume 102, pages 2032–2044, 2017

Experimental and thermodynamic investigations on the stability of $Mg_{14}Si_5O_{24}$ anhydrous phase B with relevance to Mg_2SiO_4 forsterite, wadsleyite, and ringwoodite

Hiroshi Kojitani[1,*], Saki Terata[1], Maki Ohsawa[1], Daisuke Mori[1], Yoshiyuki Inaguma[1], and Masaki Akaogi[1]

[1]Department of Chemistry, Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima-ku, Tokyo 171–8588, Japan

Abstract

High-pressure high-temperature phase relation experiments in $Mg_{14}Si_5O_{24}$ were performed using a 6-8 multi-anvil high-pressure apparatus in the pressure range of 12–22 GPa and temperature range of 1673–2173 K. We first found that $Mg_{14}Si_5O_{24}$ anhydrous phase B (Anh-B) dissociates to Mg_2SiO_4 wadsleyite (Wd) and MgO periclase (Per) at about 18 GPa and 1873 K. From the results of the high-pressure experiments, the phase boundaries of 5 Mg_2SiO_4 forsterite (Fo) + 4 Per = Anh-B and Anh-B = 5 Wd + 4 Per were determined. In addition, the isobaric heat capacity (C_P) of Anh-B was measured by differential scanning calorimetry in the temperature range of 300–770 K and the thermal relaxation method using a Physical Property Measurement System (PPMS) in the range of 2–303 K. From the measured low-temperature C_P, the standard entropy ($S^\circ_{298.15}$) of Anh-B was determined to be 544.4(2) J/(mol·K). We also performed high-temperature X-ray diffraction measurements in the range 303–773 K to determine the thermal expansivity (α) of Anh-B. The obtained C_P and α were theoretically extrapolated to higher temperature region using a lattice vibrational model calculation partly based on Raman spectroscopic data. Thermodynamic calculations by adopting the thermochemical and thermoelastic data for Anh-B obtained in this study and the estimated formation enthalpy for Anh-B of –13 208 kJ/mol gave phase equilibrium boundaries for 5 Fo + 4 Per = Anh-B and Anh-B = 5 Wd + 4 Per that were consistent with those determined by the present high-pressure high-temperature experiments. The results clarified that, in the $Mg_{14}Si_5O_{24}$ system, Anh-B is stable between 12 and 18 GPa at the expected temperatures of the Earth's mantle.

Keywords: Anhydrous phase B, phase boundary, heat capacity, entropy, thermal expansivity, Raman spectrum, wadsleyite, ringwoodite