P-V-T equation of state of hydrous phase A up to 10.5 GPa

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Abstract
Pressure-volume-temperature (P-V-T) data of synthetic Mg₇Si₂O₈(OH)₆ phase A were collected under P-T conditions up to ~10.5 GPa and 900 K by energy-dispersive X-ray diffraction using a cubic type multi-anvil apparatus, MAX80, located at the Photon Factory—Advanced Ring (PF-AR) at the High Energy Accelerator Research Organization (KEK). P-V-EoS using only room-temperature data yielded V₀ = 511.6(2) Å³, Kₐ₀ = 106.8(18) GPa, and pressure derivative Kₐ = 3.88(38). These parameters were consistent with the subsequent equation of state (EoS) analysis. The compressibility of phase A was anisotropic, with its a-axis being ~26% more compressible than the c-axis, which is normal to the plane of the distorted close-packed layers. A fit of the present data to the high-temperature Birch-Murnaghan EoS yielded V₀ = 511.7(3) Å³, Kₐ₀ = 104.4(24) GPa, K' = 4.39(48), (∂Kₐ₀/∂T)ₚ = −0.027(5) GPa K⁻¹, and thermal expansion α = a/bT with values of a = 2.88(27) × 10⁻⁵ K⁻¹ and b = 3.54(68) × 10⁻⁵ K⁻². The lattice dynamical approach by the Mie-Grüneisen-Debye EoS yielded θ₀ = 928(114) K, κ = 2.9(10), and γ₀ = 1.19(8). The isobaric heat capacity Cₚ of phase A at 1 atm. was calculated based on the Mie-Grüneisen-Debye EoS fit of present P-V-T data. In addition, the density profiles of subducting slabs with different degrees of serpentinization were also calculated along the cold geotherm up to ~13 GPa. The serpentinization of subducting slab will significantly lower the density of slab at shallower depth; however, this effect becomes negligible when antigorite dehydrates to phase A. Because the phase A bearing subducting slab is supposed to be denser than the surrounding mantle, the water can transport into deeper parts of the upper mantle and the transition zone.

Keywords: Bulk modulus, phase A, dense hydrous magnesium silicate (DHMS), equation of state (EoS), heat capacity, high pressure and high temperature (HPHT), thermal expansion; Physics and Chemistry of Earth’s Deep Mantle and Core

Introduction

Dense hydrous magnesium silicate minerals (DHMS) are potential water carriers in the deep mantle. Phase A is one group of these phases that lies on the forsterite-brucite interface in the MgO-SiO₂-H₂O (MSH) system with an ideal formula of Mg₇Si₂O₈(OH)₆. Its water content is about 12 wt%. In water-saturated peridotite system, serpentine decomposes to phase A, clinoenstatite, and water at 6.2 GPa and 853 K (Schmidt and Poli 1998). Ohtani et al. (2004) suggested that the serpentine transforms to phase A at depth greater than 180 km (~6 GPa) in a cool subducting slab, and that phase A is stable up to 11 GPa before hydrous phase E becomes the main water carrier in the slab. Komabayashi et al. (2005a) conducted experiments to examine antigorite bulk composition and pointed out that antigorite breaks down to phase A + enstatite + water at ~5 GPa, 823 K. Komabayashi et al. (2005b) also conducted experimental and theoretical study of the stability of phase A and derived the thermochemical parameters. Therefore, phase A is an important water carrier in the subduction zone after antigorite is dehydrated.

Its EoS has been of particular interest. The EoS of Fe-free phase A was reported in several studies. A range of values for bulk moduli (K₀) and the pressure derivative (K') has also been reported. Pawley et al. (1995) investigated the thermal expansivity and compressibility of phase A in the MSH system. They reported values of K₀ = 145(5) GPa (K' fixed to 4), thermal expansion α₀ = 4.9(2) × 10⁻⁵/K, and obtained the temperature derivative of bulk modulus (∂K₀/∂T)ₚ = −0.049 GPa/K using the empirical equation (∂K₀/∂T)ₚ = −7α₀. Kuribayashi et al. (2003) found that K₀ = 105(4) GPa and K' = 3.9(8) from single-crystal X-ray diffraction (XRD) up to 11.2 GPa. The Kuribayashi’s bulk modulus was markedly lower than the Pawley’s one. Crichton and Ross (2002) also measured the lattice parameters using single-crystal XRD and obtained K₀ = 97.5(4) GPa, K' = 5.97(14). The data sets from Crichton and Ross (2002) and Kuribayashi et al. (2003) are mutually consistent when considering the tradeoff between K and K'. Recently, Holl et al. (2006) studied the Fe-bearing phase A, Mg₆.₅₅Fe₀.₄₅Si₂O₈(OH)₆ using single-crystal XRD up to 33 GPa at room temperature. They reported the values of K₀ = 102.9(28) GPa and K' = 6.4(3).

In addition, Sanchez-Valle et al. (2006, 2008) determined the single-crystal elastic properties of phase A by Brillouin spectroscopy and obtained the adiabatic bulk and shear moduli and the