A new interpretation of decomposition products of serpentine under shock compression

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ABSTRACT

Dense hydrous magnesium silicates (DHMSs) may play an important role in water transport during planetary accretion and as water reservoirs in the Earth’s deep mantle. We show that the dynamic decomposition products of antigorite, Mg₅Si₄O₁₀(OH)₄, can be interpreted as containing the newly discovered, dense hydrous silicate, phase H (MgSiO₃H₂). The Hugoniot for phase H was calculated based on the Hugoniots for its constituent oxides and equation of state data derived from first-principles calculations. The measured antigorite Hugoniot, previously suggested to decompose into high-pressure phases without generating fluid H₂O, was compared with those derived from calculations involving phase H. Sound velocity data were also compared to confirm that the dynamic breakdown product of antigorite at pressures above ~40 GPa is most likely phase H plus MgO without formation of fluid H₂O.

Keywords: Dense hydrous magnesium silicates, phase H, high pressure, Hugoniot, decomposition, serpentine

INTRODUCTION

Due to their stabilities at high pressures, the dense hydrous magnesium silicates (DHMSs) may provide important insights into deep-focus earthquakes, water sources for the Earth’s interior, and formation of the primitive atmosphere and oceans (e.g., Tyburczy et al. 1990; Meade and Jeanloz 1991; Ulmer and Trommsdorff 1995; Peacock 2001; Drake 2005; Kawakatsu and Watada 2007; Sekine et al. 2012). Phase D (MgSi₂O₆H₂) previously was thought to be the only possible dense hydrous magnesium silicate present in the lower mantle (Irfune and Tsuchiya 2007). It has a wide stability field up to 40–50 GPa in pressure, at temperatures to ~1800 K, dehydrating to form an assemblage containing perovskite (Pv) and magnesiowustite (Mw) at higher temperatures (Shieh et al. 1998). Recently, using first-principles methods Tsuchiya (2013) predicted a new high-pressure hydrous phase with composition MgSiO₃H₂ as a product of a high-pressure phase transition of phase D. Subsequently, Nishi et al. (2014) observed this phase (designated phase H) experimentally at ~50 GPa and 920 °C in both quench experiments and in situ X-ray diffraction measurements using multi-anvil apparatus. At 0 K, phase H is theoretically predicted to be stable up to ~52 GPa before it dissociates into Pv plus H₂O (ice VIII) (Tsuchiya 2013). Phase H forms a solid solution with 6-Al₂O₃OH, and the stability field of the resulting alumina phase H (Al) expands to higher pressures and temperatures, extending to those that characterize the lower mantle at depths of up to ~2000 km (Nishi et al. 2014). Shock wave experiments play an important role in understanding the dynamic behavior of hydrous minerals and their stability during impact process and can be used to study their potential ability to be a water carrier.

METHOD

From theoretical calculations (Tsuchiya 2013), phase H is characterized by the zero-pressure density, bulk modulus, and its first derivative of ρ₀ = 3.412 g/cm³, K₀ = 185.8 GPa, Kʹ₀ = 4.20, respectively, although hydrogen-bond symmetrization can be expected to occur above ~30 GPa. A Hugoniot (U₁ = C₂ + sU₁, U₁ shock velocity; u, particle velocity, constants of C₀ and s) for phase H can be estimated using the equations of C₀ = (K₀ - 3) / 3 and s = (K₁ + 1) / 4 = 1.30, respectively. Moreover, phase H is compositionally a mixture of the phases brucite Mg(OH)₂ and MgO. Therefore, the Hugoniot for phase H can also be calculated based on the known Hugoniots of Br and MgO and using the additive volume law. This approach is applicable to estimate Hugoniots for an isochemical mixture of minerals with known Hugoniots (Al’-shuler and Sharipzhanov 1971; Kalashnikov et al. 1973; Telegin et al. 1980). At pressure P, the specific volume of the mineral mixture V(P) can be computed by means of the relation:

\[ V(P) = \sum_{i=1}^{n} \alpha_i V_i(P) \]

Here, \( \alpha_i \) is the weight fraction of mineral i, and

\[ \sum_{i=1}^{n} \alpha_i = 1 \]

\( V(P) \) is the specific volume of mixture i, and can be described as

\[ V_i(P) = \left( 1 - \frac{B_i - \sqrt{B_i^2 - 4A_i}}{2A_i} \right) V_{i,0} \]

(2)

Therein, \( A_i = \xi_i, B_i = 2s_i + C_{i,0}(V_{i,0}), V_{i,0}, C_{i,0}, \) and \( s_i \) are the initial specific volume, the bulk sound velocity at zero pressure, and the slope of the shock Hugoniot of mineral i, respectively. Hugoniot parameters calculated for phase H based on both the results of first-principles calculations and the additive volume law, are listed in Table 1. The calculated Hugoniots are very close to each other for P > ~40 GPa. A predicted Hugoniot for phase D (ρ₀ = 3.49 g/cm³) is also calculated from theoretical equation of state data (Tsuchiya et al. 2005), and listed in Table 1.

RESULTS

The Hugoniot for natural antigorite, Mg₅Si₄O₁₀(OH)₄, containing small amounts of Al₂O₃, FeO, and Fe₂O₃, has been determined

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