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, MgSiO3(OH)6, can be interpreted as containing the newly discovered, dense hydrous silicate, phase H (MgSiO2H2). 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 (Irifune and Tsuchiya 2000). However, serpentine containing perovskite (Pv) and magnesiowustite (Mw) at higher temperatures (Shieh et al. 1998). Recently, using 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.

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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, K0′ = 4.20, respectively, although hydrogen-bond symmetrization can be expected to occur above ~30 GPa. A Hugoniot (U = C0 + α0U, U, shock velocity, C0, particle velocity, constants of Ci and α) for phase H can be estimated using the equations of C0 = [K0 + K0′]α0 + 1/2 and α = (K0′ + 1)/4 = 1.30, respectively. Moreover, phase H is compositionally a mixture of the phases brucite Mg(OH)2(Br) plus stishovite SiO2(Si), which are stable at our pressures of interest. Therefore, the Hugoniot for phase H can also be calculated based on the known Hugoniots of Br and Si using the additive volume law. This approach is applicable to estimate Hugoniots for an isochemical mixture of minerals with known Hugoniots (Al’tshuler and Sharipdzhanov 1971; Kalashnikov et al. 1973; Telegin et al. 1980). At pressure P, the specific volume of the mixture VP can be computed by means of the relation:

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

(1)

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 mineral i, and can be described as

V_i(P) = \left(1 - \frac{B_i - \sqrt{B_i^2 - 4A_i}}{2A_i}\right) V_{i0}\n
(2)

Therein, A_i = \xi_i, B_i = 2\xi_i + C_{i0}(V_{i0}), \xi_i, C_{i0}, and \xi_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 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, MgSiO3(OH)6, containing small amounts of Al2O3, FeO, and Fe2O3, has been determined