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Determination of post-perovskite phase transition boundary up to 4400 K and implications for thermal structure in D″ layer

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ABSTRACT

We have determined the post-perovskite phase transition boundary in $MgSiO_3$ in a wide temperature range from 1640 to 4380 K at 119–171 GPa on the basis of synchrotron X-ray diffraction measurements in-situ at high-pressure and -temperature in a laser-heated diamond-anvil cell (LHDAC). The results show a considerably high positive Clapeyron slope of +13.3±1.0 MPa/K and a transition temperature of about 3520±70 K at the core–mantle boundary (CMB) pressure. The thermal structure in D″ layer can be tightly constrained from precisely determined post-perovskite phase transition boundary and the depths of paired seismic discontinuities. These suggest that temperature at the CMB may be around 3700 K, somewhat lower than previously thought. A minimum bound on the global heat flow from the core is estimated to be 6.6±0.5 TW.

1. Introduction

The thermal structure in the CMB region has profound implications for the temperature and dynamics of the core and the lower mantle. The temperature of the deep lower mantle may be around 2500 K, which is inferred by extrapolating temperature at the 660-km boundary along adiabats (Boehler, 1996). The CMB temperature (T_{CMB}) has been estimated to be approximately 4000 K based on the melting temperature of iron at the inner core boundary (Boehler, 1993). Such estimations, however, include large uncertainty, because the temperature profile in the lower mantle may be subadiabatic due to radiogenic activity (Sleep, 2003; Bunge, 2005; Zhong, 2006) and the melting temperature of iron at core pressure has been controversial (e.g., Boehler, 1993; Ma et al., 2004). The previously proposed T_{CMB} ranged from 3300 to 4200 K (e.g., Boehler, 1992; Anderson, 2002).

Recent discovery of the post-perovskite phase transition (Murakami et al., 2004; Tsuchiya et al., 2004; Oganov and Ono, 2004) has provided the first direct constraints of the thermal structure of the lowermost mantle (Lay et al., 2006; van der Hilst et al., 2007), called the D″ layer. One can expect that the lower mantle geotherm intersects the post-perovskite phase transition boundary twice due to a very steep temperature gradient in the thermal boundary layer, which is called double-crossing hypothesis (Hernlund et al., 2005). This idea was derived from the observations of paired seismic discontinuities (Thomas et al., 2004a,b). The observed depths of these paired discontinuities can tightly constrain the thermal structure in this boundary layer, if pressure–temperature (*P*–*T*) conditions of the phase transition between perovskite and post-perovskite are precisely known. In addition, a minimum heat flux across the CMB is calculated from such a temperature profile in the bottom thermal boundary layer (7.5 to 17 TW; Hernlund et al., 2005; Lay et al., 2006; van der Hilst et al., 2007), while earlier estimates of the global heat flux from the core ranged from 4 to 13 TW based on a thermal evolution and a mantle convection model (e.g., Yukutake, 2000; Labrosse, 2002; Nakagawa and Tackley, 2004; Zhong, 2006).

However, the *P*–*T* conditions of the post-perovskite phase transition are not precisely known yet (see Hirose, 2006 for a review). The transition boundary was first determined by theory (Tsuchiya et al., 2004; Oganov and Ono, 2004), but the transition pressures were different by 10–15 GPa between the GGA and LDA calculations. Previous experimental results (Murakami et al., 2004; Ono and Oganov, 2005; Hirose et al., 2006) are inconsistent with each other by more than 15 GPa, and depend strongly on the pressures scale used to calculate the pressure. Hirose et al. (2006) demonstrated that the post-perovskite phase transition occurred in $MgSiO_3$ at 119 GPa and 2400 K, matching the depth of the D″ seismic discontinuity (around 2600-km depth) (e.g., Wysession et al., 1998), based on the MgO pressure scale (Speziale et al., 2001) that is most practical at present (Fei et al., 2004). Nonetheless,

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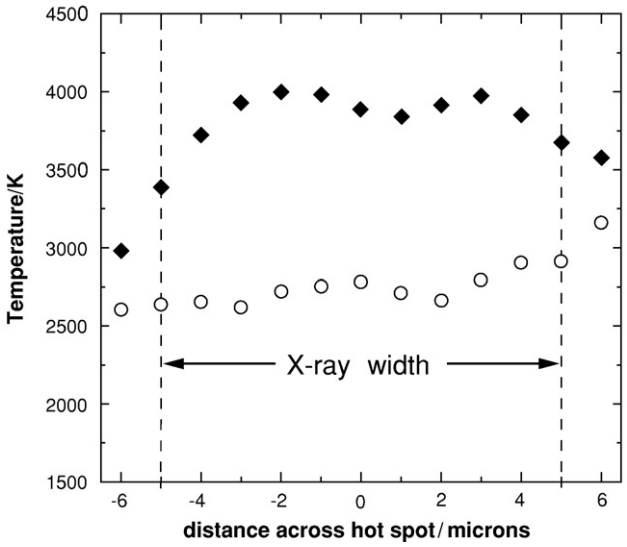

Fig. 1. Typical temperature profiles across the laser-heating spot at 129 GPa (upper) and 153 GPa (lower). X-ray diffraction was collected from the 10-μm area around the hot spot.

Hirose et al. (2006) performed experiments in a limited temperature range between 1340 and 2330 K. Since temperature error in a laser-heated diamond-anvil cell (LHDAC) was relatively large about ±10%, such a temperature range may not be broad enough to precisely constrain the Clapeyron slope and thus the boundary at higher *P*–*T* conditions remains uncertain.

Here we reexamined the post-perovskite phase transition boundary in pure $MgSiO_3$ based on in-situ X-ray diffraction (XRD) measurements in a wide temperature range between 1640 and 4380 K at pressures of 119 to 171 GPa. The results show a very high positive Clapeyron slope of +13.3 MPa/K and the temperature intercept, T_{int} (transition temperature at the CMB pressure) of about 3500 K. These suggest a relatively low T_{CMB} and small heat flow from the core.

2. Experimental techniques

High *P*–*T* conditions were generated using the LHDAC techniques. We prepared a gel starting material with a chemical composition of $MgSiO_3$, which was dehydrated by heating to 1273 K before experiment. It was mixed with an MgO powder for an internal pressure standard. The sample mixture was pressed to a disc with a thickness of ~20-μm and coated with a thin film (~100-nm thick) of gold (runs #1, 2, and 4) or rhenium (run #3) for both sides that served as a laser absorber. It was placed into an ~50-mm hole drilled in a rhenium gasket, and subsequently argon was cryogenically loaded into a sample chamber. These were compressed with beveled diamond anvils with 150- or 200-μm culet. We heated the sample with TEM_{01*}-mode Nd:YLF laser using double-sided heating technique that minimizes axial temperature gradient within the sample (Shen et al., 1996). Temperature was measured by the spectroradiometric method.

Angle-dispersive XRD spectra were collected on a CCD detector (Bruker APEX) at BL10XU of SPring-8 (Ohishi et al., in press). Exposure time was 5 to10 s. A monochromatic incident X-ray beam with a wavelength of 0.4125–0.4128 Å was collimated to 10-μm in diameter. Two-dimensional XRD images were integrated as a function of two-theta angle in order to have conventional one-dimensional diffraction profiles using the fit-2D program (Hammersley, 1998). The uncertainty in temperature within the 10-μm area from which X-ray diffractions were collected was less than ±10% even above 4000 K (Fig. 1). Pressure was determined from the unit-cell volume of MgO using its *P*–*V*–*T* equation of state proposed by Speziale et al. (2001), which is the same as that used in our previous study (Hirose et al., 2006). The pressure errors at high temperatures were ±1.5–4.3 GPa, arising mainly from the large uncertainties in temperature when calculating the *P*–*V*–*T* equation of state. In runs #1 and #2, heating cycles were repeated with increasing/decreasing the load pressure (Table 1). The diffraction patterns of the sample were collected at high temperatures and at room temperature before and after the heating cycles (Fig. 2).

3. Results

We have conducted four separate sets of experiments at pressures between 119 and 171 GPa and temperatures up to 4380 K (Table 1). In the first set of experiment (Fig. 3a), the starting material was compressed to 102 GPa at room temperature (Fig. 2a) and subsequently heated to 2890 K at 123 GPa. The orthorhombic perovskite (space group: *Pbnm*) was immediately formed from the amorphous sample. When temperature was increased to 3750 K at GPa, perovskite peaks further grew (Fig. 2b). After quenching to room temperature, this sample was further compressed and reheated to 3680–3960 K at 139–144 GPa. The diffraction peaks of post-perovskite (space group: *Cmcm*) appeared in 2 min, while perovskite peaks became weak with time (Fig. 2c). In the following heating cycle performed at 136 GPa, 1640 K and 146 GPa, 2560 K, we observed further growth of post-perovskite peaks relative to those of perovskite (Fig. 2d). We then reduced the pressure at 300 K and reheated the sample to 3200 K at 145 GPa. The peaks from post-perovskite became

Table 1
Experimental *P*–*T* conditions and results on pure $MgSiO_3$[a]

Run	Cycle	a_{MgO}[b] (Å)	*P* (GPa)	*T* (K)	Observation as grown phase
1	1	3.7771	122.9 (26)	2890	Pv
		3.7809	129.1 (34)	3750	Pv
	2	3.7559	139.4 (34)	3680	PPv
		3.7515	144.0 (37)	3960	PPv
	3	3.7216	136.1 (15)	1640	PPv
		3.7184	146.4 (25)	2560	PPv
	4	3.7339	145.1 (31)	3200	PPv
2	1	3.6971	158.5 (26)	2690	PPv
	2	3.7032	169.1 (40)	4100	PPv
		3.7049	171.0 (43)	4380	PPv
	3	3.7450	149.3 (40)	4200	Pv
	4	3.7732	131.7 (34)	3680	Pv
	5	3.7780	119.0 (23)	2520	Pv
3		3.7383	133.2 (20)	2170	PPv
		3.7448	135.8 (26)	2750	PPv
4		3.7553	140.2 (35)	3730	Pv+PPv

[a] Number in parenthesis indicates uncertainties in the last digits. PPv, post-perovskite; Pv, perovskite.
[b] Pressure are calculated using the MgO scale of Speziale et al. (2001).