EARTH & PLANETARY SCIENCE

Lattice thermal conductivity of MgSiO₃ perovskite and post-perovskite at the core-mantle boundary

Heat in the Earth's interior is transported dominantly by convection in the mantle and core, and by conduction at thermal boundary layers. The thermal conductivity of the bottom thermal boundary layer of the mantle determines the magnitude of heat flux from the core, and is intimately related to the instability of the boundary layer and the formation of mantle plumes, the thermal evolution of both the mantle and the core, and driving force for generation of the geomagnetic field [1]. Core heat loss can be estimated quantitatively from the temperature gradient in the boundary layer and the thermal conductivity of the lowermost mantle. However, the thermal conductivity has been poorly constrained at high pressure. The lattice thermal conductivity and related thermal diffusivity of $MgSiO_3$ perovskite (Pv), a primary mineral in the Earth's lower mantle, have only been measured at 1 bar and 26 GPa [2,3]. Its pressure dependence therefore remains uncertain. The value of $MgSiO_3$ post-perovskite (PPv), a high-pressure polymorph of $MgSiO_3$ Pv, has only been speculated. Previous estimates of the lower mantle thermal conductivity range widely between 5 and 30 W/m/K, with a typical value being 10 W/m/K [1,4].

In this study [5], we determined the lattice thermal conductivity of $MgSiO_3$ Pv and PPv over the entire lower mantle pressure range of up to 144 GPa and at room temperature by means of a newly developed pulsed light heating thermoreflectance technique in a diamond-anvil cell (DAC) (Fig. 1(a)). We used polycrystalline $MgSiO_3$ Pv as a sample, which was synthesized in a multi-anvil apparatus prior to the thermal diffusivity measurements. Since complete transformation from Pv to PPv was found to be difficult when using Pv as the starting material, we also used $MgSiO_3$ gel as the starting material for the measurements of PPv. The sample plate was coated with sputtered platinum (Pt) film on both sides for laser heating and thermoreflectance measurement. It was loaded into a hole in a rhenium gasket, together with NaCl layers that served as both a pressure medium and thermal insulator (Fig. 1(a)). Before each thermoreflectance measurement, the sample was annealed by heating with a multi-mode Nd:YAG laser or two 100 W single-mode Yb fiber lasers to ~1800 K, except below 22 GPa. PPv was synthesized directly from the gel starting material by heating with the fiber lasers to 2000 K for 60 min. The high-intensity monochromatic X-ray beam at beamline **BL10XU** enabled us to obtain high-resolution X-ray diffraction (XRD) patterns from the sample, in which we could observe sharp XRD peaks from $MgSiO_3$ Pv or PPv (Fig. 1(b) for example).

After phase identification by synchrotron XRD measurements, the lattice thermal diffusivities of both Pv and PPv were measured in a DAC by the thermoreflectance technique. A $50-100$ μm area of the Pt film was heated from one side by a pulsed Nd:YAG laser with a pulse duration of 2 ns. The applied heat was conducted through the sample to the Pt film on the opposite side. The temperature rise after pulse heating was monitored as a change in reflectivity of the Pt film (Fig. 1(c)). The reflectivity was probed using a linearly polarized continuous-wave diode laser (782 nm in wavelength). The obtained transient
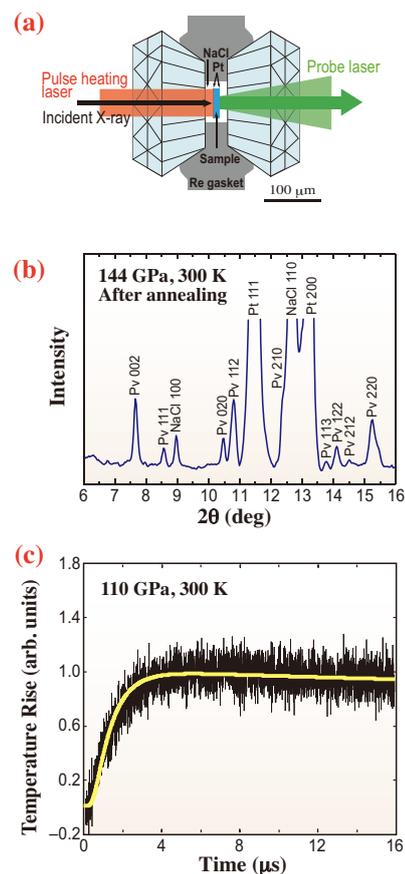

Fig. 1. **(a)** Schematic drawing of sample configuration. A monochromatic incident X-ray beam was collimated to about a 6 μm area on the sample (black arrow). Angle-dispersive XRD spectra were collected on a CCD detector at BL10XU before the thermoreflectance measurements. After pulse laser heating of Pt film on one side (red), the heat was transported by conduction through the sample to the Pt film on the other side. This heat diffusion time was determined from the change in reflectivity of the latter Pt film, which was monitored using a continuous-wave laser (green). **(b)** Representative XRD pattern of $MgSiO_3$ Pv at 144 GPa and 300 K after thermal annealing. **(c)** Transient temperature curves for $MgSiO_3$ Pv at 110 GPa and room temperature. Yellow curve shows fitted result.

temperature curves, such as that in Fig. 1(c), were analyzed considering one-dimensional heat diffusion to determine the heat diffusion time of the sample (see [5] for details). The thickness of both the sample and the Pt foils at high pressure was estimated after the thermoreflectance measurement. We determined the thermal diffusivity of Pv and PPv at high pressures from the heat diffusion time and the sample thickness obtained in this study, and then calculated the lattice thermal conductivity of Pv and PPv at high pressures as the product of their thermal diffusivity, density, and heat capacity at constant pressure.

We conducted ten separate experiments to measure the lattice thermal diffusivities of $MgSiO_3$ Pv from 11 to 144 GPa at room temperature. As plotted in Fig. 2, the thermal diffusivity of Pv varied with increasing pressure; it increased from 2.5 ± 0.2 mm^2/s at 11 GPa to 11.6 ± 2.5 mm^2/s at 144 GPa. In addition, we measured the lattice thermal diffusivities of $MgSiO_3$ PPv at 135 and 141 GPa at room temperature. The diffusivities of PPv at 135 and 141 GPa were 19.0 ± 4.4 mm^2/s and 20.0 ± 4.6 mm^2/s, respectively, which were 72% greater than those of Pv at equivalent pressures (Fig. 2). The calculated conductivities of Pv and PPv were 9.0 ± 1.6 and 16.8 ± 3.7 W/m/K, respectively, at 135 GPa and 3700 K, which corresponds to the proposed condition at the core–mantle boundary (CMB) (Fig. 3(a)). We also computed the bulk lattice thermal conductivity of an 80 vol% $MgSiO_3$ Pv and 20 vol% MgO periclase (Pe) mixture using the recent results for Pe [3] (Fig. 3(b)). Our results yielded a Pv-dominant lowermost mantle conductivity of about 11 W/m/K, which is comparable to the conventionally assumed value of 10 W/m/K. We also found that PPv-bearing rock exhibits 60% higher conductivity than Pv-dominant rock.

The bulk lower mantle thermal conductivity has been conventionally assumed to be about 10 W/m/K [4]. The lattice thermal conductivity of Pv+Pe rock (4:1 mixture for pyrolitic lower mantle) estimated above is
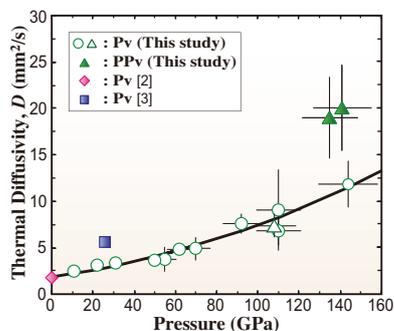
consistent with this value, and therefore, our findings do not indicate any significant increase or decrease relative to previously employed values. Because all previous calculations of heat flow for the PPv double crossing assumed a lowermost mantle conductivity of 10 W/m/K, compatible with the value for Pv obtained in this study, the present findings do not significantly alter the magnitude of CMB heat flow implied by this model. Indeed, the present results support the notion of high CMB heat flow (46.6 TW) along with a high degree of secular core cooling, and are in accord with the idea of an extensively molten lowermost mantle in Earth's distant past [1].
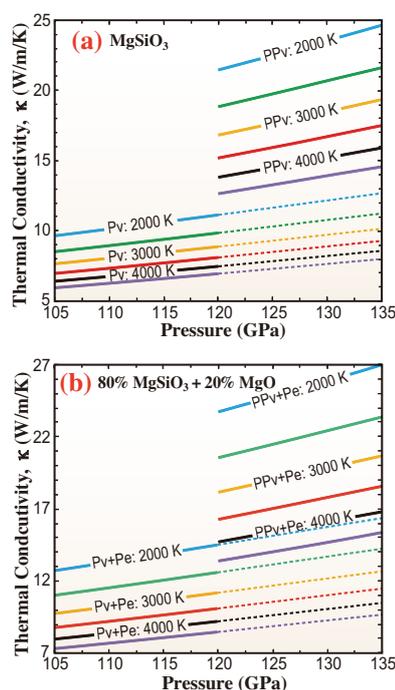
Fig. 3. Lattice thermal conductivity (κ) of deep lower mantle. 4:1 mixture of $MgSiO_3$ Pv/PPv and Pe [3]. Isotherms are at 500 K intervals between 2000 and 4500 K. The uncertainty of present estimates is about 20%.

Fig. 2. Lattice thermal diffusivity (D) of $MgSiO_3$ Pv and PPv at high pressure and 300 K. Circles: Pv (samples synthesized in a multi-anvil apparatus, this study); open triangle: Pv at 108 GPa (sample synthesized from gel starting material in a DAC, this study); diamond: Pv at 1 bar [2]; squares: Pv at 26 GPa [3]; filled triangles: PPv (this study).

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