Toward precise thermal/chemical modeling of lower mantle

The lower mantle is the largest part in the solid Earth, and composes more than 50% of the volume and mass. Therefore, the chemical composition of the lower mantle has a great influence on the bulk composition of the planet. The chemical composition of the upper mantle is well known to be peridotitic on the basis of geological evidence. Hence, if we know the chemical composition of the lower mantle, we can estimate the material recycling and chemical differentiation history in the mantle from the difference between the chemical compositions of the upper and lower mantle. In addition to its abundance, the lower mantle has other important features. The lower mantle consists of silicate and oxide, and it has much lower thermal conductivity and higher viscosity than the metallic liquid outer core, which is the second largest convecting part in the solid Earth. Thus the lower mantle can be considered as a thermal insulator controlling the cooling history of the solid Earth. In the material recycling and cooling history, convection is the most important mechanism, and pressure-volume-temperature equations of state (P-V-T EOS) and the knowledge of the thermodynamic properties such as thermal expansion coefficients and heat capacities of constituent materials are essential for understanding the mantle convection.

$MgSiO_3$ is the most abundant end component of the dominant lower mantle phase, magnesium-rich silicate perovskite. Therefore, numerous reports of high-pressure and high-temperature in situ X-ray diffraction studies of $MgSiO_3$ perovskite using synchrotron radiation sources can be found in the literature, indicating that the thermoelastic properties of $MgSiO_3$ perovskite are constrained. However, thermal properties remain uncertain because of uncertainties in pressure scales and/or differences in high-pressure techniques. In order to clarify these uncertainties, we carried out high-pressure and high-temperature in situ measurements for $MgSiO_3$ perovskite based on a large-volume high-pressure technique developed at **BL04B1** using a multianvil apparatus "SPPED-Mk.II" [1], and at **BL10XU** using a laser-heated diamond anvil cell. In addition, we used a new EOS of MgO, which was determined from pressure-scale-free experimental data, as a primary pressure scale for static high-P,T experiments [2].

Using two high-pressure devices with one of the most reliable pressure scales, P-V-T EOS and thermodynamic properties of $MgSiO_3$ perovskite were precisely determined on the basis of robust experimental results obtained in the entire stability field of $MgSiO_3$ perovskite up to 110 GPa and 2500 K (Fig. 1; Ref. [3]). The new EOS of $MgSiO_3$ perovskite is consistent with that of MgO. In addition to the magnesium-rich silicate perovskite, ferropericlase (magnesiowüstite) is another main phase in the lower mantle, and MgO is the dominant end component making up more than 80 mol% of the ferropericlase in pyrolitic bulk composition (e.g., Ref. [4]). The comprehensive P-V-T EOS and thermodynamic properties of $MgSiO_3$ perovskite and MgO determined in this study will play a critical role in the mineralogical and thermal modeling of the Earth's lower mantle.

Figure 2 shows comparisons of calculated density and adiabatic bulk modulus values and those observed using the geophysical model known as PREM [Dziewonski and Anderson, 1981]. Here, the density and adiabatic bulk modulus were calculated referring to the model geotherm of Brown and Shankland (1981). Absolute values of density are tightly constrained within the uncertainty of 0.01 g/cm at most for both $MgSiO_3$ perovskite and MgO (Fig. 2(a)). The densities of $MgSiO_3$ perovskite and MgO are much lower than those obtained by PREM owing to a lack of iron in the system. When we carry out mineralogical modeling, we must take into account the effects of iron incorporation on mass and volume in both $MgSiO_3$
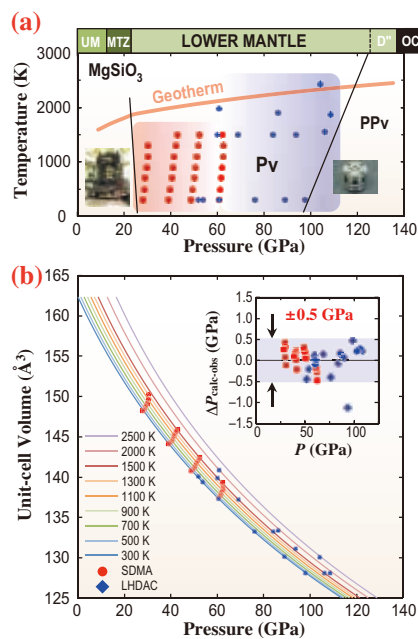

Fig. 1. Measured P, T conditions with phase relation in $MgSiO_3$ **(a)**, and P-V-T data along with the isotherms at 300-2500 K **(b)**. Red circles and blue diamonds represent the results obtained in the experiment using sintered-diamond multianvil apparatus (SDMA) and laser-heated diamond anvil cell (LHDAC). Inset in (b) shows differences between measured data and determined EOS model.
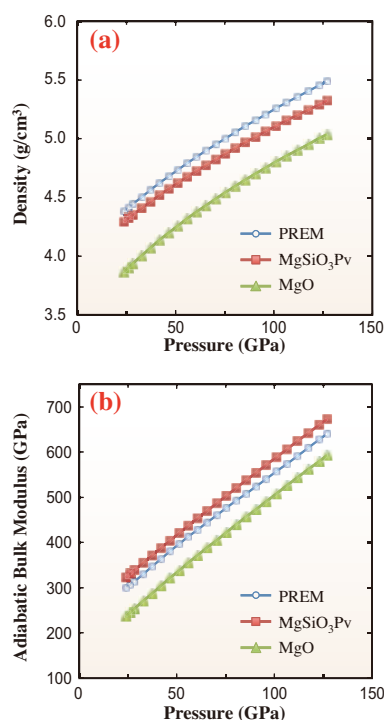
Fig. 2. Density **(a)** and adiabatic bulk modulus **(b)** of MgSiO$_3$ perovskite and MgO, compared with PREM. Error bars for those properties are smaller than the symbol size.

perovskite and MgO, and also on Fe-Mg partitioning between (Mg,Fe)SiO$_3$ perovskite and (Mg,Fe)O. The volume increase in perovskite due to Fe-incorporation and Fe-Mg partitioning of (Mg,Fe)SiO$_3$ perovskite and (Mg,Fe)O was already investigated at BL04B1 using a sintered-diamond multianvil apparatus [4,5], and the results will be merged in the lower mantle modeling in the near future. In addition, the adiabatic bulk modulus is also precisely determined with the uncertainties of less than 5 GPa up to 100 GPa (Fig. 2(b)). In order to improve current EOS models, precise high-temperature (2000 K) elastic measurements (±5 GPa in uncertainties) are required at pressures in the Mbar region. In the case of the bulk modulus of perovskite, the effect of iron incorporation is known to be marginal, and current results are applicable to the mineralogical modeling up to the Mbar region. On the other hand, although the effect of iron incorporation is complicated in ferropericlase because of the spin-state transition in ferrous iron, its effects on density and thermoelastic properties will be clarified using the results for MgO as a reference. Consequently, the newly established comprehensive adiabatic bulk moduli of MgSiO$_3$ perovskite and MgO support a bulk pyrolitic lower mantle rather than a perovskite-rich composition. If we employ a bulk perovskite composition, extraordinarily high temperatures (additional > 1000 K) are required to reproduce the K_S observed seismologically, because of a small $\partial K_S/\partial T$ of MgSiO$_3$ perovskite (~0.02 GPa/K) in the deep lower mantle.

In addition to applications to chemical modeling, current EOS models can contribute to the thermal model of the lower mantle. The lower mantle is considered to be convecting and thus its temperature profiles would be close to adiabatic. The adiabatic temperature profile is derived by integrating a fundamental thermodynamic relationship, $(\partial T/\partial P)_S = \alpha V T/C_P$ or $(\partial T/\partial P)_S = \gamma T/K_S$, where α, C_P, and γ are the thermal expansion, isobaric heat capacity, and Grüneisen parameter, respectively. The integrating operation requires one reference P-T condition, and Fig. 3 shows a result obtained with the reference temperature of 1900 K at 23 GPa, corresponding to a depth of 660 km in the Earth. The present EOS models of MgSiO$_3$ and MgO yield intermediate temperature profiles compared with previous models proposed of Brown and Shankland (1981) and Anderson (1982), and they are rather close to that by Stacey and Davis (2004). Our new EOS models give the current CMB potential temperature between 2570 K and 2750 K. In the near future, the temperature profile and the mineralogical model will be refined comprehensively using the present EOS as standards, and hopefully will provide insights on the chemical differentiation and cooling history of the solid Earth.
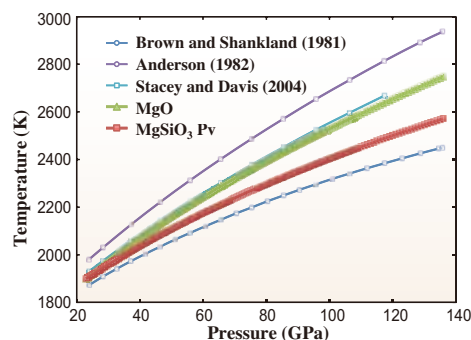

Fig. 3. Adiabatic temperature profiles derived using current EOS models of MgSiO$_3$ and MgO under lower mantle conditions and previous models proposed by Brown and Shankland (1981), Anderson (1982), and Stacey and Davis (2004).

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