Consideration of decomposition of CaSiO3-perovskite based on the equation of state of CaO

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CaSiO3-perovskite is one of the important constituent minerals in the lower mantle. There is a possibility that CaSiO3-perovskite may decompose into CaO + SiO2 in the lower mantle. This is because the cell volume CaSiO3-perovskite is slightly smaller than the total volume of CaO + SiO2 in the pressure condition of the lower mantle. There is report that MgSiO3-perovskite decomposed into MgO + SiO2 (Saxena et al, 1996). In this study, we discussed a possibility of decomposition of CaSiO3-perovskite by comparison between the density of CaSiO3-perovskite and that of CaO + SiO2. P-V-T equation of state of CaO have been investigated using in situ diamond-anvil X-ray diffraction technique, and samples were heated by Pr-Rh heater.

1. Introduction

It is thought that CaSiO3-perovskite is one of the important constituent minerals in the lower mantle.CaSiO3-perovskite may exist as CaO + SiO2(stishovite) in the lower mantle. There is a report that MgSiO3-perovskite decomposed into MgO + SiO2(stishovite) from the latest research. Although this report has not been confirmed by other researchers, it is thought that CaSiO3-perovskite may also decompose into CaO + SiO2(stishovite). The B1 to B2 transition of CaO occurs at about 60-70GPa, and the volume decreases about 11 percent. If the lattice structure of CaO was B2 structure, volume of CaO + SiO2(stishovite) is almost the same as that of CaSiO3-perovskite.That is, it is thought that CaSiO3-perovskite may not exist but CaO(B2 structure) + SiO2(shishovite) in the lower mantle. In this study, we discussed a possibility of decomposition by comparison between volume of CaSiO3-perovskite and that of CaO + SiO2(stishovite).

2. Experiment

The sample was prepared from CaCO3 heated for 4 hours at 1550K. Since CaO was easy to absorb water, it was immediately mixed after composition in the silicon grease that is a pressure medium. In situ X-ray powder diffraction measurement under high temperature and high pressure using external heated diamond anvil cell was carried. External heated DAC is composed of a Pt-Rh(40) line as a resistance heating element, 0.25 carat diamonds as anvil, Re sheet as a gasket, and Alumel-Chromel thermocouple for measurement of temperature. Ruby fluorescence method was used for measurement of pressure at ambient temperature, and Au was used at high temperature. Runs were made with a X-ray generator with a Mo rotating anode operated at 50kV and 150mA.Imaging Plate(RIGAKU R-AXIS4++) was used as a X-ray detector, and analysis of IP data was carried using PIP as a software of analysis. Calculation of lattice constants were carried by reading peak top of diffraction pattern at ambient temperature, and using profile fitting at high temperature.

3. Result and Discussion

The transition pressure from B1 to B2 structure is 60.8GPa at 295K, and 61GPa at 583K. This means the phase boundary of B1 to B2 transition is dominantly dependent on pressure. It is thought that this is because the volume change accompanied by a phase transition is extremely large. Moreover, fitting of Birch-Murnaghan equation of state was performed to the obtained data. Bulk modulus of B1 structure is 125(1)GPa at 295K, 123(1)GPa at 488K, and 122(1)GPa at 584K.(first-order pressure derivative of bulk modulus is fixed to 3.6) Bulk modulus of B2 structure is 140(20)GPa at 295K, 136(20)GPa at 485K, 132(20)GPa at 584K, and 128(20)GPa at 685K. .(first-order pressure derivative of bulk modulus is fixed to 4) Moreover, temperature dependence of bulk modulus and thermal expansion at ambient pressure were calculated. The calculated values were used for extrapolation to the lower mantle condition. The data of Wang et al(1996) is used for CaSiO3-perovskite, and that of Liu et al(1999) is used for SiO2(stishovite). Pressure, which the latter volume become smaller than the former volume, is about 85GPa at 1000K, and 60GPa, 2000K. It is thought that CaSiO3-perovskite may decomposed into CaO+SiO2(stishovite) in volume in lower mantle conditions from this result.