Structural Phase Transition in SiO_2

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1 Introduction

Silica, SiO_2, is a major mineral in the subducted oceanic plate. Therefore, the physical properties associated with the phase transitions of silica play an important role in understanding the composition, structure, and dynamics of the earth's mantle. Moreover, its polymorphic transitions from quartz to coesite and from coesite to stishovite have been extensively used for pressure calibrations at high pressures and high temperatures, such as for $CaGeO_3$ [1], Fe_2SiO_4 [2], $MgSiO_3$ [3], and Mg_2SiO_4 [4]. Determination of the phase diagram for silica is therefore of particular interest to the study of the high-pressure behaviors of materials.

2 Experiment

The starting material was SiO_2. High-pressure X-ray diffraction experiments were performed using a multi-anvil high-pressure apparatus. The cubic anvil assembly was compressed using a "Max III" high-pressure apparatus, and was combined with a synchrotron radiation source located at the KEK in Japan. We also used experimental data from SPring-8, which is similar facility of PF-AR. The diffracted X-rays were detected using a germanium solid-state detector at an angle of $2\theta = 6.0°$. A cylindrical TiB_2 heater was inserted into the octahedral pressure medium and enclosed within a ZrO_2 sleeve for thermal insulation [1,2]. The powdered sample and gold, which was used as pressure calibrant, were loaded directly into the TiB_2 heater, which also served as a sample capsule. The pressure was determined from the unit cell volume of gold using the equation of state for gold. After reaching the required temperature, we performed in situ measurements using the synchrotron X-rays. The duration of heating was 1-4 hours. Determination of the stable phase in each experimental run was carried out by observing the X-ray diffraction pattern of the sample. To check the identification of each phase in the in situ experiments, the recovered samples were also examined using micro Raman spectroscopy.

3 Results and Discussion

We performed approximately 30 experimental runs to investigate the phase boundary between coesite and stishovite [5]. The P-T conditions of the acquired X-ray diffraction patterns and the stable phases identified are shown in Fig. 1. The gradient of dP/dT of the phase boundary was positive. The transition boundary shown in Fig. 1 is represented by the following linear equation:

$$P \text{ (GPa)} = 4.7(3) + 0.0031(2) \times T \text{ (K)}.$$

The boundary determined in this study is in general agreement with those reported in previous in situ high-pressure experiments. However, the dP/dT slope was more positive than that in the previous in situ experiments. The estimated value of the dP/dT slope using the thermodynamic calculation is consistent with that determined in our study.

The phase transition between coesite and stishovite at ~10 GPa, i.e., ~300 km depth, might be related to the observed seismic X-discontinuity. The transition pressure determined in our study is in good agreement with that corresponding to the depth of the X-discontinuity.
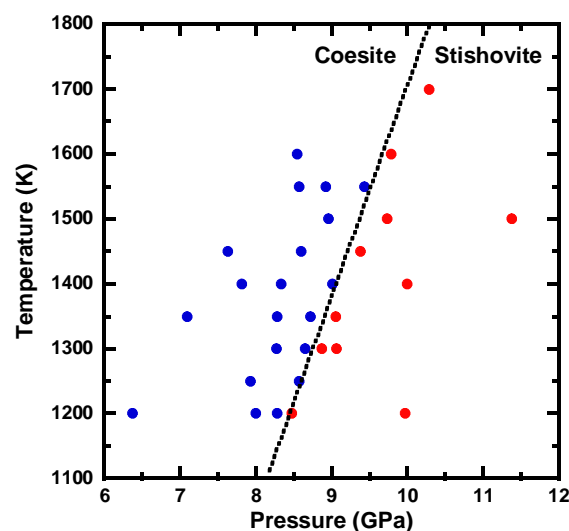

Fig. 1: Experimental results and phase boundary of the coesite-stishovite transition in SiO_2.

Acknowledgement

References

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