High Pressure X-ray Diffraction Study on $CaSnO_3$ Perovskite

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Perovskite-structured silicate (orthorhombic, space group Pbnm, hereafter called Pv) is demonstrated to be the dominate phases in the Earth's lower mantle. Recently, a phase transition from perovskite structure to post-perovskite structure in $MgSiO_3$ was discovered at ~125 GPa corresponding to the core-mantle boundary region (D" layer) (Murakami et al.,2004). The post-perovskite is a $CaIrO_3$-type structure (orthorhombic symmetry, space group Cmcm, hereafter called PPv). General regards that the pv-ppv phase transition in Mg-silicate is the best explanation of geophysical anomaly near the D" layer.

Due to the extreme high P-T conditions of pv-ppv phase transformation in Mg-silicate, it's difficult to study the physical properties of ppv-silicate experimentally. Alternatively, the perovskite-structured analogues are used to conduct the experiments for the first-order study on the physical properties of PPv structure. Lately, the first-principles calculation (Tsuchiya and Tsuchiya, 2006) suggested that perovskite-structural $CaSnO_3$ could transform into post-perovskite structure at 12GPa.

In this study, we used the high pressure techniques to explore the high pressure phase transition in $CaSnO_3$ perovskite experimentally. The high-pressure conditions were generated in a diamond-anvil cell (DAC). Angle-dispersive X-ray diffraction spectra were collected on imaging plate (IP). The results of $CaSnO_3$ perovskite have been collected up to 25 GPa based on NaCl pressure marker along compression and decompression as shown in Fig. 1.

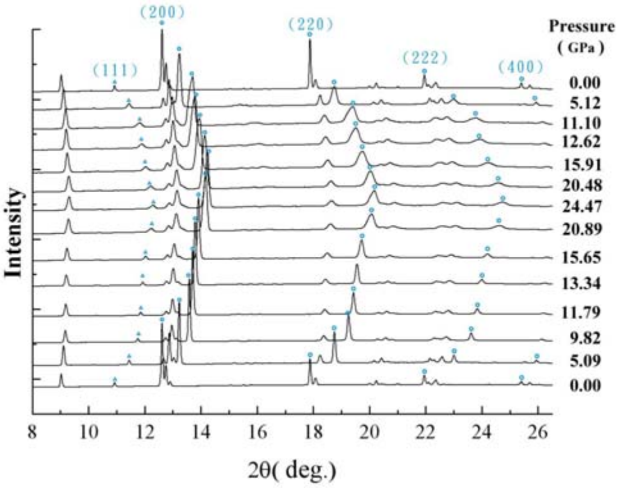

Figure 1. Selected X-ray diffraction patterns of $CaSnO_3$ pv and NaCl (blue markers) at different pressures. The pressure scales on the right were calculated based on equation of state of NaCl.

The determination of unit cell parameters of $CaSnO_3$ perovskite and NaCl pressure marker were refined using the program package GSAS (General Structure Analysis System, Larson and Von Dreele, 1988). As starting models for refinement in the Rietveld mode at different pressure conditions, then the final values of lattice parameter were obtained by a Le Bail refinement (Le Bail et al., 1988) in which least-square fitting of the diffraction profiles was achieved by minimization of the difference between the observed and synthetic patterns. During the refinement , the X-ray diffraction patterns for $CaSnO_3$ perovskite specimen were remaining pretty similar throughout the whole pressure range. We did not observe any extra peak appeared or peak disappeared in the entire of experiment. The resultant unit-cell parameters and cell volume of $CaSnO_3$ perovskite were shown in Fig. 2 (plotted as a/a_0, b/b_0, c/c_0 and V/V_0 v.s. pressure), a continuous decreasing function as pressure increased. From above evidence, we found no phase transition occurred in $CaSnO_3$ perovskite up to the pressure covered in this study.

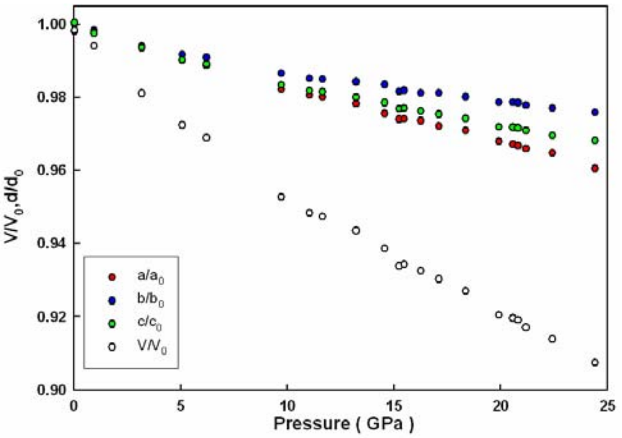

Figure 2. Variation of a/a_0, b/b_0, c/c_0 and V/V_0 of $CaSnO_3$ perovskite with pressure at room temperature.

We have experimentally studied the phase transition in $CaSnO_3$ perovskite at high pressure that it was predicted to have Pv-PPv transition at 12 GPa by computation. X-ray diffraction technique is sensitive to the change in crystal structure. Based on the X-ray diffraction study, we found that crystal structure of $CaSnO_3$ reminds perovskite phase from sambient conditions up to the the peak experimental pressure of 25 GPa. We conclude that there is no pressure-induced phase transition occurred in $CaSnO_3$ perovskite up to 25 GPa, room temperature.