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Effect of the incorporation of $Fe^{3+}AlO_3$ into $MgSiO_3$ perovskite on the phase transition to post-perovskite

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Introduction

$MgSiO_3$ perovskite is thought to be the most abundant mineral phase in the Earth's lower mantle. Recently the post-perovskite transition was discovered at the P-T conditions just above the core-mantle boundary [1]. This transition has received much attention because the D" layer located at the bottom of the lower mantle is possibly explained by the post-perovskite phase of $MgSiO_3$. It has been known that the incorporations of ferric iron and aluminum into perovskite possibly influence the transition pressure to the post-perovskite phase. The increase of aluminum content in $MgSiO_3$ expands the stability field of perovskite toward higher pressure as the experimental and the theoretical studies confirmed [2,3]. On the other hand, there is a theoretical report that the incorporation of ferric iron into $MgSiO_3$ decreases the transition pressure to post-perovskite [4]. Although the *ab intio* simulation predicted that the incorporation of $Fe^{3+}AlO_3$ lowered the post-perovskite transition pressure, the theoretical calculation in Fe-bearing system has not been established still enough [5]. Therefore the experimental approach is significantly requested to understand the transition pressure in the $MgSiO_3$-$Fe^{3+}AlO_3$ system.

Experiments

The starting material was prepared as a gel with $Mg_{0.85}Fe^{3+}_{0.15}Al_{0.15}Si_{0.85}O_3$ composition. The starting material was mixed with a fine powder of gold as a pressure standard for in-situ X-ray experiments [6]. The sample was sandwiched between NaCl pellets and loaded into a hole of Re gasket. The samples were heated from both sides with YAG or YLF laser. Temperature was measured from one side by the spectrodiometric method.

Synchrotron X-ray diffraction measurements were carried out at high pressures and a room temperature in the beam line 13A and 18C. The monochromatic incident X-ray beams with a wavelength of about 0.42 Å and 0.61 Å were collimated to 15-20 μm in diameter. X-ray diffraction spectra were recorded with an imaging plate.

Results and Discussion

The starting material was compressed to 117 GPa at room temperature, and then heated at 1600 K for an hour. After heating, temperature was quenched to room temperature. An *in-situ* X-ray diffraction pattern was measured at 115 GPa and 300 K. All diffraction peaks except reflections derived from NaCl and gold can be indexed as the orthorhombic perovskite with space group *Pbnm*. The unit cell parameters of perovskite are refined from 15 independent reflections and are a = 4.334(1) Å, b = 4.601(1) Å, c = 6.312(1) Å. Pressure was further applied to ~143 GPa and ~2500 K. Perovskite is also stable phase at these conditions.

At 157-160 GPa and 1600-2500 K, perovskite and post-perovskite could be observed. The perovskite and the post-perovskite phases stably coexist at these conditions. Although the chemistry of the coexisting phases could not be measured, the X-ray diffraction patterns of the sample behave as the product phase in the pseudo-binary system of $MgSiO_3$-$Fe^{3+}AlO_3$.

A single phase of post-perovskite was finally observed at 175 GPa and 1600 K. The unit cell parameters of post-perovskite are a = 2.430(1) Å, b = 7.896(5) Å, c = 6.045(2) Å at 172 GPa and 300 K. The $Fe^{3+}AlO_3$-bearing post-perovskite phase transformed to the amorphous state on the process of releasing pressure, and this evidence is the same phenomenon as observed in pure $MgSiO_3$ post-perovskite.

Pure $MgSiO_3$ perovskite transforms to the post-perovskite phase at 113 GPa and 2400 K with a positive Clapeyron slope of 4.7 MPa/K [7]. However, the present study shows that the perovskite phase with $Mg_{0.85}Fe^{3+}_{0.15}Al_{0.15}Si_{0.85}O_3$ is solely stable at least up to 143 GPa and 2500 K. Moreover, we observed the coexistence of perovskite and post-perovskite at about 160 GPa and a single phase of post-perovskite could be finally observed at about 180 GPa. These results strongly suggest that the incorporation of 15 mol% $FeAlO_3$ into $MgSiO_3$ perovskite expands the stability field of the perovskite phase toward higher pressure by more than about 40 GPa.

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