Effect of FeO and Al2O3 on post-perovskite phase transiton in MgSiO3

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The recent experimental and theoretical studies have found that the orthorhombic MgSiO3 perovskite (space group: Pbnm) transforms to a CaIrO3-type post-perovskite phase (Cmcm) above 125 GPa and 2500 K nearly corresponding to the top of D" layer. In natural mantle composition, incorporation of FeO, Fe2O3, and Al2O3 to MgSiO3 perovskite and post-perovskite should be took into consideration. In order to know the effect of FeO and Al2O3 on the post-perovskite phase transition, we investigated phase relations in (Mg0.5Fe0.5)SiO3 and Mg3Al2Si3O12 on the basis of in-situ synchrotron X-ray diffraction measurements at high-pressure and -temperature in a laser-heated diamond anvil cell (LHDAC).

In the system of (Mg0.5Fe0.5)SiO3, results demonstrate that perovskite was formed as a single phase up to 108 GPa at 2200 K, indicating that (Mg,Fe)SiO3 perovskite accommodates significant amounts of FeO at such high pressures. Both perovskite and CaIrO3-type post-perovskite coexisted above 107 GPa at 1500 K, the condition very close to the post-perovskite phase transition boundary in pure MgSiO3. The coexistence of perovskite and post-perovskite was observed, at least to 123 GPa. The post-perovskite-in curve in (Mg0.5Fe0.5)SiO3 is very close to the post-perovskite phase transition boundary in pure MgSiO3. Contrary to earlier experimental and theoretical studies, these results show that the incorporation of FeO expands the stability of perovskite relative to post-perovskite. This could be due to a larger ionic radius of Fe2+, which is hard to substitute the small Mg2+ site in the post-perovskite phase. Furthermore, in the system of Mg3Al2Si3O12, we observed that single perovskite is solely stable up to 140 GPa and 2200 K, and perovskite and CaIrO3-type post-perovskite phase coexist above 140 GPa and 2200 K. Post-perovskite is formed as a single phase above 150-170 GPa. Previous study has shown that pure MgSiO3 perovskite transforms to post-perovskite phase above 125 GPa and 2500 K based on the same pressure standard [Murakami et al., 2004]. Our results indicate that incorporation of both FeO and Al2O3 expands the stability of MgSiO3 perovskite relative to post-perovskite.