

Phase relations and structure variations of CaSiO₃-CaTiO₃ perovskites under high pressure and high temperature

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CaSiO₃ has a cubic or pseudocubic perovskite structure at high pressure and high temperature, and it is thought to be one of the major constituent minerals of the lower mantle. Meanwhile CaTiO₃ has an orthorhombic perovskite structure in the wide pressure and temperature region, and is sometimes used as analogue material for MgSiO₃ perovskite also considered to be the major constituent mineral of the lower mantle. Therefore, the study of the phase relations and structure variations of the system CaSiO₃-CaTiO₃ is important to understand the crystal chemistry of Ca-perovskites and also the crystallochemical behaviors of CaSiO₃ perovskite in the lower mantle. For such purposes CaSiO₃-CaTiO₃ perovskites were synthesized by high pressure and high temperature experiments including a multianvil cell and a laser-heated diamond anvil cell, and the product phases were analyzed by synchrotron X-ray diffraction, small-area X-ray diffraction and analytical electron microscopy.

Analyses of the quenched products of the multianvil cell experiments showed that perovskite was the only existing phase in the whole area of this system above 12.5 GPa at 1773 K, and perovskite was orthorhombic (Pbmn) for the region from CaTiO₃ to about 40 mol percent CaSiO₃, and it had a double perovskite-like structure whose unit cell is double of CaSiO₃ cubic perovskite for the region from about 40 mol percent to 65 mol percent CaSiO₃, and for the region from 65 mol percent to endmember CaSiO₃ the quenched specimens were amorphous. There was no two-phase region of perovskites.

Meanwhile in-situ synchrotron X-ray diffraction experiments of this system using a laser-heated DAC at 30 GPa and 1800 K showed that perovskite in the intermediate composition showed peaks of double perovskite where indices were all even or all odd, indicating a face-centered cubic lattice. But the recovered specimens at room temperature showed the extra peaks which violate a face-centered cubic lattice. These results combined with the observation by ATEM indicate that Ca(Si,Ti)O₃ perovskite in the intermediate composition is double perovskite with a face-centered cubic lattice under high pressure and high temperature, but it inverts to the lower symmetry phase with a simple cubic lattice by the Si-Ti ordering during quenching.