Post-stishovite phase transition mechanism of SnO2 by high-pressure single-crystal X-ray diffraction study

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Stishovite is one of the dominant phases in lower mantle and its physical properties might be very important to comprehend the mantle science. SiO2 stishovite (rutile-type structure, P42/mnm) has been reported to transform to CaCl2-type structure (Pnnm) at about 50 GPa, to alpha-PbO2-type structure at (Pbcn) 120 GPa, and further to pyrite-type structure (Pa-3) at about 200 GPa (Andrault et al. 1998). SnO2 is an analogue material to SiO2, but the phase transition from rutile structure to CaCl2 is expected to occur at considerably lower pressures.

In the present study the post-stishovite phase transition of SnO2 has been conducted by a high-pressure single-crystal X-ray diffraction study. A cramp-type diamond-anvil cell was used for high-pressure experiments at room temperature using a 16:3:1 methanol-ethanol-H2O mixture as the pressure medium. And the ruby fluorescence technique was applied for pressure estimation. X-ray diffraction intensity measurements with MoKa radiation were made using a four-circle diffractometer.

In stishovite phase, the shared O-O distance for octahedron is considerably compressible than the other O-O distances and apical Sn-O[2] distance is less compressible than the equatorial Sn-O[4] bond distance. With increasing pressure the destabilization of rutile-type structure is induced from on their short-range coulomb interactions. We found the twinned texture composed of alpha-PbO2 due to the transition from CaCl2 structure at 15GPa under nonhydrostatic conditions. Under hydrostatic conditions, this twin was not observed, and CaCl2-pyrite transition twin was observed at 20GPa. We assume that CaCl2-type phase can be directly transform to the high-pressure phase of pyrite without intermediate phase of alpha-PbO2 which might be metastable phase.

Recently, a higher-pressure form named by orthorhombic-I (Pbca), was found by Shieh et al. (2006) above 50GPa during room-temperature compression. But our experiment was carried out below 40GPa, orthorhombic-I phase was could not observed.