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Thermodynamic study of perovskite - post-perovskite transition of CaIrO3

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CaIrO3 post-perovskite is an analogous material of MgSiO3 post-perovskite. CaIrO3 post-perovskite is thermodynamically stable at ambient conditions. CaIrO3 perovskite also can be obtained as a metastable phase. Therefore, we can make calorimetry of both of them. Thermodynamic interpretation of the perovskite - post-perovskite phase transformation of CaIrO3 will give us useful information to understand that of MgSiO3. As CaIrO3 hardly dissolved in both lead borate and sodium molybdate solvents, a solution enthalpy measurement could not be employed. In this study, we tried to determine an enthalpy of CaIrO3 perovskite - post-perovskite transformation using the decomposition reaction of CaIrO3 into CaO + Ir + O2 above 1513 K at 1atm.

CaIrO3 post-perovskite was prepared by calcining the mixture of CaCO3 and IrO2 with the composition of CaCO3 : IrO2 = 1:1 in mole ratio at 1173 K for 2 hours and heating at 950 ºC for 3 hours in air. CaIrO3 perovskite was synthesized by keeping a staring material of CaIrO3 post-perovskite at 1.5 GPa and 1673 K for one hour by using a Kawai-type high-pressure apparatus at Gakushuin University. High-temperature drop calorimetry was performed using the SETARAM MHTC calorimeter. Powdered sample was put in a Pt capsule and dropped into the calorimeter at 1573 K. Weights of sample and Pt capsule were 20 mg and 60 mg, respectively. An observed enthalpy was calibrated by alumina as a standard.

Observed enthalpies for post-perovskite and perovskite phases were determined to be 486.7+/- 9.2 kJ/mol (8 data) and 454.5 +/- 10.8 kJ/mol (7 data), respectively. From the difference between them, the phase transition enthalpy from perovskite phase to post-perovskite phase was obtained to be -32.2 +/- 14.2 kJ/mol. A Clapeyron slope of the phase boundary between those phases was calculated to be dP/dT = 50 +/- 20 MPa/K, if the phase boundary was fixed at 1.5 GPa and 1648 K which were determined by our high-pressure experiments. The result of the thermodynamic calculation in this study suggests that the phase boundary of CaIrO3 post-perovskite phase transition has considerably large positive Clapeyron slope.