Lattice dynamical implication of ilmenite MgXO3 (X=Si, Ge, Ti) using Raman spectroscopy at high-pressures and high-temperatures

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Ilmenite-type MgX4+O3 have various stable P-T region due to their composition: MgSiO3-, MgGeO3- and MgTiO3-ilmenite is stable at high-pressures, moderate-pressures and ambient pressure, respectively. In this study, we conducted a high-pressure, high-temperature Raman spectroscopic study of ilmenite-type MgSiO3, MgGeO3 and MgTiO3. From the viewpoint of elasticity and bonding energy, we investigate the behavior of ilmenite at high-pressure and high-temperature and compare structures of ilmenites that have different compositions.

Raman spectroscopy was a triple microspectrometer equipped with an optical microscope and an Ar ion laser. High-temperature experiments were performed using a Pt-electric resistant heater. For the high-pressure experiments, a diamond-anvil cell (DAC) was used using H2O as the pressure media. Raman spectra of each sample were collected up to 770 K at ambient pressure and 30 GPa at room temperature, respectively.

From the obtained Raman bands, we calculated the force constant, k, of the stretching mode (Ag(1) and Eg(1)) and obtained the temperature and pressure dependence of k. The temperature dependence of k was the order of Ge-O, Si-O and Ti-O stretching bands. The tendency induces the relative expansion rate for each XO6 (X=Si,Ge,Ti) octahedron. This is consistent with the fact that MgTiO3 ilmenite is the only stable phase phase at the present HT experimental conditions. On the other hand, the order of the pressure dependence of k is complex. For Si-O and Ge-O bonds, the pressure dependence of k of Ag(1) is larger than that of Eg(1). Namely, shorter X-O bonds (Ag(1)) are more shortened under pressure than longer X-O bonds (Eg(1)), indicating that the distortion of XO6 octahedra is enhanced at higher pressures. For Ti-O bond, the contrary pressure dependence was observed. These phenomena obtained are consistent with the results of the single-crystal structure analyses by Yamanaka et al. (2003, submitted).