High-pressure, high-temperature Raman spectroscopic study of ilmenite-type MgSiO₃, MgGeO₃ and MgTiO₃

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Poster Presentation at AGU (American Geophysical Union) 2004 fall meeting
Location: Moscone Convention Center, San Francisco, California, USA
Date: December 13-17, 2004
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Ilmenite-type MgSiO₃ is a high-pressure polymorph of enstatite, and characterized by a relatively narrow stability field in the 20-24 GPa and 1370-2270 K range. Since MgSiO₃-ilmenite is stable at thermodynamically low temperature, it is considered to be a candidate component in 600-700 km of subducting slabs. It is important for earth science to understand its crystal structure on the basis of lattice vibrations at high pressure and temperature. High-pressure and high-temperature Raman spectra of ilmenite-type MgSiO₃ have already been collected up to 7 GPa and 1030 K, respectively (Reynard and Rubie, 1996). 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 NRS2100 triple microspectrometer equipped with Ar ion laser (operating at 514.5 nm and 70-80 mW). High-temperature experiments were performed using a Pt-electric resistant heater. Temperature was monitored with chromel-alumel thermocouples. For the high-pressure experiments, a diamond-anvil cell (DAC) was used. H₂O was preferred to an alcohol mixture as the pressure media because it has no strong Raman bands in the measured region. Pressures were determined from the shift of the ruby fluorescence R₁ line, excited by the Ar ion laser. Raman spectra of each sample were collected up to 770 K at ambient pressure and 30 GPa at room temperature, respectively.

For ilmenite, 10 bands were expected from symmetry analysis (five A_g and five E_g). At ambient conditions, we could observe seven (for MgSiO₃), eight (for MgGeO₃) and nine (for MgTiO₃) Raman bands, respectively. With increasing temperature, each band shifted to lower wavenumber. The temperature dependence of the force constant, k, was the order of MgGeO₃, MgSiO₃ and MgTiO₃. 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 up to 770 K at ambient pressure in this study. With increasing pressure at room temperature, each Raman band shifted to higher wavenumber. We also discuss the pressure dependence of the force constant, k.