In situ XAFS study on pressure-induced local structure change of SrGeO3 melt

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The structural and physical properties of silicate melts are very important for understanding the evolution and dynamics of the Earth's interior. However, in situ structural studies of silicate melts up to the high-pressure region where structural changes are expected to occur have not been successful to date because of experimental difficulties. Using a high-pressure XAFS technique, we have investigated the local structure of Li2Ge4O9 melts and demonstrated that a dense liquid phase with GeO6 octahedron appears under pressure. Liquid germanates is the closest structural analogue of liquid silicates (magma). In this study, we have investigated the local structure of SrGeO3 melt using a high-pressure and high-temperature XAFS technique.

High-pressure and high-temperature XAFS experiments were performed at SPring-8 beamline BL14B1 using multianvil high-pressure apparatus. SrGeO3 powder was mixed with B2O3 and BN, and put in a BN sample chamber. B2O3 was used to lower the melting temperature and suppress the decomposition of SrGeO3. BN was used to dilute the sample for XAFS measurements. Pressure transmitting medium was boron and epoxy resin. A pair of LaCrO3 disk was used for a heater. Temperature was monitored by a W-Re thermocouple. Generated pressure was estimated using the calibration curve based on NaCl pressure scale. XAFS spectra near Ge K-edge with an energy range of 1000 eV above the edge were successfully measured up to 10 GPa at 1573 K.

The first neighbor Ge-O distances in SrGeO3 measured at room temperature show an abrupt increase between 3 and 5 GPa corresponding to the coordination number change of Ge atoms from 4 to 6. The Ge-O distance of the melt measured at 3 GPa is consistent with that of crystalline phase at 3 GPa and increases with compression over 5 GPa. We conclude that the fourfold coordination is dominant up to 3 GPa in the present melt.