

Structural behavior of silicate liquids and glasses under extreme conditions by using synchrotron X-ray diffraction and Raman spectroscopy

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The behavior of silicate melts under high-pressure and high-temperature conditions is of primary interest in the field of geophysical, chemical, material science, and technological glass process industry, both for their fundamental properties and for their significant roles in thermal transport and chemical differentiation within Earth and other terrestrial planetary interiors. In order to understand the origin and significance of deep melts in Earth's interior, it is important to obtain laboratory constraints on thermodynamics properties of silicates under extreme conditions. However, despite their crucial roles in dynamic processes, little is known about the nature of liquid silicates and glasses properties throughout the Earth's pressure regime because the high-pressure and high-temperature environment entails severe experimental difficulties. Recently, considerable progress has been achieved in understanding the structural differentiation of liquid and glass silicates by both theoretical predictions and various spectroscopic experiments, yet still many issues are puzzling and several challenges must be overcome to expand our understanding of silicate liquids and glasses. Here, we report spectroscopic properties of hedenbergite ( $\text{CaFeSi}_2\text{O}_6$ ), diopside ( $\text{CaMgSi}_2\text{O}_6$ ), wollastonite ( $\text{CaSiO}_3$ ), enstatite ( $\text{MgSiO}_3$ ), and silica ( $\text{SiO}_2$ ). The local atomic structure of various silicates has been studied using synchrotron angle-dispersive X-ray diffraction combined with a multi-channel collimator. Atomic pair distribution functions (PDFs) were obtained from the X-ray data. Also, we have obtained the local vibrational modes by using Raman spectroscopy, providing additional structural information that cannot be obtained by X-ray diffraction. The results allow us to contribute better understanding of the structure-property relationships to silicate melts and glasses, providing important implication for the evolution of deep Earth's interiors.