Structure of silicate glasses up to 172 GPa

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Abstract

The physical properties of silicate melts at temperature and pressure conditions of the Earth's mantle have a fundamental influence on the chemical and thermal evolution of the Earth. However, direct investigations of melt structures at these conditions are experimentally very difficult or even impossible with current capabilities. In order to still be able to obtain an estimate of the structural behavior of melts at high pressures and temperatures, amorphous materials have been widely used as analogue materials.
Here we report experimental investigations of the structural behavior of glasses of SiO2 up to 172 GPa, MgSiO3 up to 135 GPa, and Mg2SiO4 up to 140 GPa using X- ray total scattering and pair distribution function analysis. To further understand ultra high pressure behavior we have investigated GeO2 glass, as an analogue for SiO2 glass, up to 85 GPa. The very high pressure range for these measurements were enabled by the newly commissioned multichannel collimator setup at GSECARS, APS, which significantly reduces the amount of diamond Compton scattering. This facilitates the collection of total x-ray diffraction patterns up to a maximum Q of 15 A-1 at very high pressures.

The data clearly shows changes from 4- to 6-fold coordination of Si, which is completed around 40-60 GPa, depending on composition, in agreement with previous reports. GeO2 shows an increase to 6-fold coordination already about 25-30 GPa. At higher pressures, after the change to 6-fold coordination, the glasses show smooth changes in structure factors S(Q) and pair distribution functions g(r). The Si coordination number gradually increases to about 7.2 at 172 GPa for SiO2 with no apparent discontinuity.
We will present experimental data, discuss densification mechanisms and differences of the various glass compositions at high pressures. The goal is to establish a framework for silicate glass structures as analogue materials for silicate melts to understand the deep Earth's interior.

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