Structural relaxation of high pressure Ca aluminosilicate melts during quenching and decompressio

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Transportation of magma in the Earth's interior is controlled by density and viscosity, which are strongly connected with the structure of magma. Structural study of magma is, therefore, fundamental to elucidate physical properties of magma. Pressure-induced structural change of magma has been studied by glasses quenched from melts under pressure. Recently, Allwardt et al. (2005), however, reported that recovered glasses do not possess the structure of high pressure melt due to structural relaxation during quenching and decompression. It is, therefore, necessary to understand the detail of structure relaxation process, in order to understand structure of silicate melt under high pressure. In this work, we investigate relaxation process during quenching and decompression, based on X-ray diffraction analysis and MD simulation of $Ca_3Al_2Si_6O_{18}$ composition high pressure melt, quenched glass, and decompressed glass.

High pressure and high temperature in-situ X-ray experiments have been carried out by using cubic-press MAX80 installed at PF-AR NE5C of KEK. X-ray diffraction patterns of melt and glasses were acquired by energy dispersion method with white X-ray up to 7.0GPa and 2100K. We also used MD simulation to reproduce the structure of $Ca_3Al_2Si_6O_{18}$ melt and glasses, to compare the results of X-ray structure analysis.

X-ray structure analysis revealed some structural changes during quenching both in radial distribution function and in interference function, which are attributed to abrupt increase of coordination number of Al around glass transition temperature 1500K and to gradual increase of coordination number of Ca by MD simulation. X-ray structure analysis also shows peak height change of the FSDP during quenching. The peal intensity of the FSDP, however, does not change during quenching, indicating that the change of the peak height is not correlate to the intermediate-range order but is simply affected by thermal vibration. MD simulation, however, shows that T-O-T angle changes with decreasing temperature above 1500K, implying the change of bonding of TO_4 tetrahedra. During decompression, MD simulation can not reproduce the structural relaxation because of limited time of MD simulation, and it accounts for elastic deformation only. According to X-ray structure analysis, the expansion of inter-atomic distance during decompression is larger than that evaluated from MD. Thus structural change during decompression may include the short-range structure change, such as decrease of nearest neighbor coordination number.