

Static structure of hydrous magnesium silicate melt under high-pressure and high-temperature

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Structures of hydrous magnesium silicate melts ($Mg/Si=1.8$ and 2.0 at $8-9$ GPa, $1750K$) and $MgSiO_3$ glass (up to 14.7 GPa, $600K$) were investigated by high-pressure X-ray diffraction experiments using synchrotron radiation. The interference function and the radial distribution function were derived from the several diffraction data. As the result, the first-neighbor distances r_{Si-O} of the present hydrous magnesium silicate melts were 1.68\AA in both the melt composition of $Mg/Si=1.8$ and that of $Mg/Si=2.0$. These results may show that SiO_4 tetrahedron, which is a fundamental structure unit of silicate melt and glass, change to polyhedron which has higher coordination number, CN, from $CN=4$ to 5 at around 9 GPa. On the other hand, Si-Si distance r_{Si-Si} corresponding to the distance between SiOn polyhedrons had big difference between two hydrous magnesium silicate melts with the composition of $Mg/Si=1.8$ and with the composition of $Mg/Si=2.0$. r_{Si-Si} of the melt with $Mg/Si=1.8$ was 3.11\AA , and that of the another melt with the composition of $Mg/Si=2.0$ was 2.94\AA . This difference shows that SiOn polyhedrons exist independently or not in those melts. Polyhedrons in the melt with the composition $Mg/Si=2.0$ were not polymerized because Mg_2SiO_4 forsterite ($Mg/Si=2.0$) has independent structure in terms of tetrahedrons. Thus the melt has the similar structure to its crystal phase. On the other hand, the melt with the composition of $Mg/Si=1.8$ is richer in composition of Si than $Mg/Si=2.0$, therefore it has some network structures in terms of SiOn polyhedrons.

Reliability of the present analysis was confirmed comparing the present result of $MgSiO_3$ glass at ambient condition with that of Waseda and Toguri (1990), which report the result of $MgSiO_3$ melt using angle-dispersive x-ray diffraction method at room pressure, $2000K$. These were consistent each other, and the present analyses was found to be suitable. The result of $MgSiO_3$ glass at 14.0 GPa, $600K$ shows that the change of r_{Si-Si} is larger than that of r_{Si-O} with increasing pressure; this suggests that the structure changes between SiO_4 tetrahedrons involve densification of $MgSiO_3$ glass at least up to 14.0 GPa, $600K$.