Pressure-induced structural change in magnesium silicate melts

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First principles calculation using periodic boundary conditions and density functional theory on high-performance computers have made great achievements in materials science under extreme conditions. However, many difficulties related to the dynamics and the size effects arise when it is extended to aperiodic systems such as liquids and amorphous solids under high temperature and high pressure [1]. Nonetheless the remarkable improvement of hardware capabilities and invention of new algorithms in the scope of the post-post-K computers will promote discoveries of new physics of such liquids.

Recently, a glass-glass transition of $MgSiO_3$ was observed at 88 GPa and room temperature using X-ray diffraction measurement under static compression in a diamond anvil cell[2]. It was suggested that this transition may be extended to a liquid-liquid transition of $MgSiO_3$ melt at higher temperatures and pressures, which corresponds to the perovskite post-perovskite (Pv-PPv) transition of $MgSiO_3$ crystal [3, 4].

Shock compression experiments for $MgSiO_3$ [5, 6] and Mg_2SiO_4 [7, 8]melts have been also performed making it possible to explore the structure and properties of liquids directly.

In this presentation, we report the results of molecular dynamics simulation of magnesium silicate melts under high temperature and high pressure using various simulation schemes such as Empirical Potential Molecular Dynamics (EPMD) [9]and First Principle Molecular Dynamics (FPMD) simulation[10] as well as Large-scale First Principle Molecular Dynamics (L-FPMD) simulation for a consistent understanding.

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