Structures and properties of liquids in the deep Earth

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The physical and chemical properties of condensed matters (solids and liquids) are determined by their microscopic atomic structures. Although the atomic structures can generally be determined by various experimental measurements, it encounters many experimental difficulties with liquids under extreme environments such as high pressure and high temperature. Nonetheless, development of new experimental techniques and construction of next generation synchrotron radiation facilities are expected to further elucidate the structure and physical properties of liquids (magma, liquid iron) in the deep Earth.

On the theoretical side, the crystal structure prediction methods using high-performance computers have made great achievements in material sciences under extreme conditions such as earth science, super-hard materials and high-temperature superconductivity [1, 2]. Since the method is based on the periodic system at absolute zero temperature, 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. 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 in such liquids. I will review several examples of such efforts related to the size effect and the nano-heterogeneity [1, 2].

References

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