

Structure of water under high pressure: expectations for neutron scattering

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Water is the most important liquid for our life so that it is studied in many fields such as biology, earth and environment sciences, medicine, engineering, chemistry and physics. Water is also special because it has anomalous properties that are different from those of ordinary molecular liquids. These anomalies are attributed to a remaining hydrogen-bond network structure formed by four-fold coordinated water molecules. Pressure is supposed to change such an open-packed structure drastically. We have studied structure of liquid (fluid) water by in-situ high-pressure high-temperature x-ray diffraction measurements using multi-anvil presses at BL04B1 and at BL14B1 in SPring-8 synchrotron radiation facility. We have found that the coordination number of water molecules increases rapidly to about 10 around 4 GPa. The structure of water evolves toward a simple structure which can be described by a hard sphere model with increasing pressure.

In the x-ray diffraction, hydrogen atoms, which have only one electron, barely contribute diffraction intensity. Hence the contribution of the oxygen-oxygen pair dominates in the radial distribution function and information about hydrogen bonds, which play an important role in the structure of water, cannot be deduced. In contrast to the x-ray diffraction, neutron diffraction is a powerful tool to investigate hydrogen atoms because hydrogen atoms have a large cross section to neutrons. In fact, several neutron diffraction studies have been done for water at ambient and relatively low pressures. In this talk, a brief review of our synchrotron radiation study, previous neutron diffraction and simulation studies for water under high pressures will be given. What we expect in the future neutron scattering studies under high pressure will be discussed.