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Temperature dependence of structure of water

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Liquid water at ambient conditions shows unique properties because of hydrogen-bonded network structure. We conducted high-pressure high-temperature x-ray diffraction experiments up to 17 GPa at the SPring-8 synchrotron radiation facility and reported that the local structure changed towards a simple liquid-like structure through an increase of coordination number up to 4 GPa [1]. The increase of the coordination number saturates around 4 GPa and intermolecular distance decreases on further compression. However these data were measured just above the melting temperature at each pressure so that the effect of pressure (density) and that of temperature could not be separated. In this work, we have conducted x-ray diffraction measurement at various temperatures keeping the density around 1 g/cm³. The measurements were conducted using a cubic-type multi-anvil press installed on BL14B1 at the SPring-8. There is a unique double peak structure in structure factor, $S(Q)$, of water. It is related to the characteristic local structure. This double peak structure almost vanishes at 200 °C. This result suggests a structural change from a low coordinated structure to a simple liquid-like structure. Effects of density and temperature on structure of water will be discussed.

[1] Y. Katayama, T. Hattori, H. Saitoh, T. Ikeda, K. Aoki, H. Fukui, and K. Funakoshi, Phys. Rev. B, 81, 014109 (2010).

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