Atomic- and molecular-structural measurement of highly supercompressed liquid water at room temperature by using dynamic diamond anvil cell

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Investigating mysterious properties of water requires detailed understanding of its structural evolution as a function of controllable thermodynamic parameters. By using an advanced dynamic diamond anvil cell unit in conjunction with in-situ X-ray diffraction and micro-Raman spectroscopy, we measured atomic- and molecular-level structural evolution of highly supercompressed liquid water well beyond its equilibrium melting pressure of ice-VI phase up to the deep metastable region, in which ice-VII is likely to form at room temperature. Our structural factor data shows continuous increase and sharpening of the first peak, whereas intensity of the secondary peak progressively decreases. We also observe that the first peak moves toward higher Q signaling decrease in the intermolecular distance as pressure increases. While the disappearance of the characteristic double peak feature (Q = 1.5 ~ 3.5 A-1) typically implies loss of open tetrahedral network structure as reported at elevated temperatures, our Raman spectral data shows that frequencies of the OH-stretching band modes decrease with pressure indicating the strengthening of the hydrogen bonds. Such a capability to measure structural evolution of liquid in deep metastable states is very important for understanding various crystallization behaviors in water.

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