SHOCK19-2019-000744

Abstract for an Invited Paper
for the SHOCK19 Meeting of
the American Physical Society

Unraveling the exotic properties of water ices with laser-driven compression and x-ray diffraction[1]

FEDERICA COPPARI, LLNL

Since Bridgmans discovery of five solid water (H2O) ice phases in 1912, studies on the extraordinary polymorphism of H2O have documented more than seventeen crystalline and several amorphous ice structures, as well as rich metastability and kinetic effects. This unique behavior is due in part to the geometrical frustration of the weak intermolecular hydrogen bonds and the sizeable quantum motion of the light hydrogen ions. Particularly intriguing is the prediction that H2O becomes superionic [1]with liquid-like hydrogens diffusing through the solid lattice of oxygen when subjected to extreme pressures exceeding 100 GPa and temperatures above 2000 K. Numerical simulations of superionic water ice suggest that the characteristic diffusion of charged hydrogen ions through the oxygen solid lattice should not only enable a surprisingly high ionic conductivity, but it should also dramatically increase its melting temperature to several thousand Kelvin and favor new ice structures having a close-packed oxygen lattice. Because confining such hot and dense H2O in the laboratory is extremely challenging, experimental data are scarce. Recent optical measurements along the Hugoniot curve of water ice VII showed evidence of superionic conduction and thermodynamic signatures for melting, but did not confirm the microscopic structure of superionic ice [2]. I will discuss recent experiments at the Omega Laser using laser-driven shockwaves to simultaneously compress and heat liquid water samples to 100400 GPa and 20003000 K. In situ X-ray diffraction measurements show that under these conditions, water solidifies within a few nanoseconds into nanometer-sized ice grains that exhibit unambiguous evidence for the crystalline oxygen lattice of superionic water ice. The X-ray diffraction data also allow us to document the compressibility of ice at these extreme conditions and a temperature- and pressure-induced phase transformation from a body-centered-cubic ice phase to a novel face-centered-cubic, superionic ice phase, which we name ice XVIII [3]. In addition to representing a critical test to numerical method for high pressure/high temperature condensed matter, the experimental discovery of superionic water ice at conditions expected deep inside ice giant planets provides new constraints to planetary models describing the interior structure or Uranus and Neptune

[1] Cavazzoni et al. Science 283, 4446 (1999)
[2] Millot et al. Nat. Phys. 14, 297302 (2018)
[3] Millot et al. Nat. 569, 251 (2019)

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.