Phase transition of two-dimensional water/ice in graphene nanocapillaries

Y.B. Zhu,[*] F.C. Wang, H.A. Wu

Department of Modern Mechanics, University of Science and Technology of China, China.

*Presenting author: zhuyinbo@mail.ustc.edu.cn

Abstract

Water and ice are omnipresent on Earth and ubiquitous on comets, planets, and planet moons. On earth, unconstrained water typically exhibits vapor, liquid, and solid (ice I_h) forms. However, when constrained in nanoscale environment and under ultrahigh pressure, water and ice manifest dramatic differences from their bulk counterparts in part because the van der Waals pressure can induce water-to-ice transformation, known as the metastability limit of the two-dimensional (2D) liquid. From mechanics point of view, the liquid-to-solid transformation characterizes the compression limit of 2D water. In many applications, evaluation of the metastability stability of a solid under conditions of tension or compression is often performed to provide mechanical property that is critical for structure design and assessment. Here in, we illustrate the phase transition of 2D water/ice constrained in graphene nanocapillaries. At 300 K, myriad of 2D ice polymorphs, including monolayer, bilayer and trilayer crystalline-like ices or amorphous ices, are formed from the liquid water at different width of the nanocapillaries, ranging from 6.0 Å to 11.6 Å. The compression limit (phase) diagram is obtained at the nanocapillary width *versus* pressure (h-P) plane, based on the comprehensive molecular-dynamics simulations at numerous thermodynamic states as well as on the Clapeyron equation. Interestingly, the compression-limit curves exhibit multiple local minima, reflecting the metastability (phase) diagram. Moreover, our further simulation studies reveal that lateral pressure can be used as a key controlling parameter to realize first-order and continuous-like phase transitions in the compression and superheating limits of confined 2D water/ice.

Keywords: confined water, graphene nanocapillaries, compression limit, phase transition, molecular dynamics simulation