Effect of Electric Field on the Behaviors of Phase and Phase Transition of Water Confined in Carbon Nanotube

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ABSTRACT In our previous work, we have found that liquid water can freeze continuously into either pentagonal or helical solid-like ice nanotube in a single-walled carbon nanotube (SWCNT) (diameter=1.2 nm), depending on the strengths of the external electric field (*E*) applied along the tube axis. In this study, we have investigated the structure and the phase transition behavior of water confined in a thicker SWCNT (diameter=1.31 nm) by performing molecular dynamics simulations at atmospheric pressure. We found that confined water can freeze into three different polygonal ice nanotubes through a first-order phase transition at lower E (<1.25 V/nm), and form a helical ice nanotube encapsulating a helical water nanoline through a continuous phase transition at higher E (1.25 V/nm < E <2 V/nm). The boundaries of the two different phase transitions are connected by a connecting point. The populations of the three different polygonal ice nanotubes are modulated by both temperature and electric field. In addition, an E-induced discontinuous structure transition between polygonal and helical ice nanotubes is observed at low temperature with a large electric hysteresis loop of 1.0 V/nm. Finally, we propose a rich phase diagram of confined water in the temperature-electric field plane.