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Controllable Mechanical Property and Deformation Response of Water-Filled Carbon Nanotubes under Electric Field

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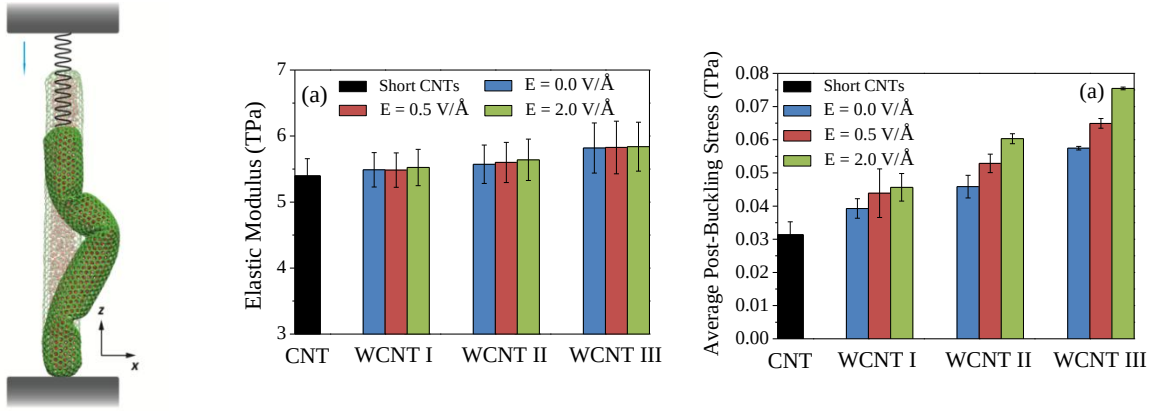
Many previous works focused on the effect of filling on the mechanical, electrical and optical properties of carbon nanotubes (CNTs).[1,2] It is well known that water is a typical incompressible fluid composed of polar molecule, which can provide uniform and powerful internal supports for the CNTs. However, although the water-filled CNTs have been fabricated in the laboratory,[3] the researches on the mechanical property of water-filled CNTs still lack. In this work, the mechanical property and deformation response of water-filled CNTs are studied by molecular dynamics (MD) simulations.

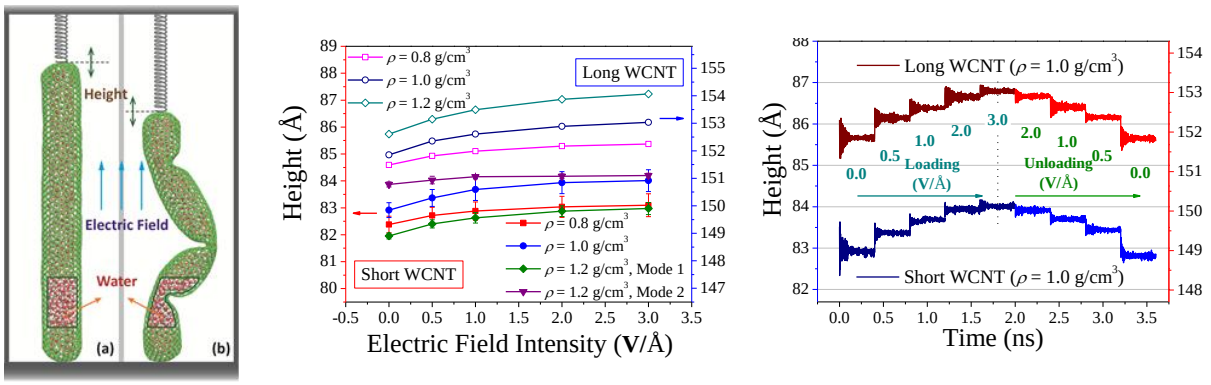


(a) MD model (b) Elastic modulus (c) Average post-buckling stress

Fig.1 The mechanical property of water-filled CNTs

Figure 1 gives the MD model, elastic modulus and average post-buckling stress of water-filled CNTs. The MD model is constructed by a capped (12, 12) CNT filled with water molecules (Fig. 1(a)). The bottom cap of the water-filled CNT is fixed, and the top cap is compressed by a moving spring. The simulation results indicate that the water filling and

electric field can result in a slight change in the elastic property (the elastic modulus (Fig. 1(b)) and Poisson's ratio) of the water-filled CNTs. However, the yield stress and average post-buckling stress (Fig. 1(c)) exhibit a significant response to the water density and electric field intensity.



(a) MD model (b) Height change (c) Time response

Fig.2 The deformation response of water-filled CNTs

Figure 2 shows the MD model, height change with electric field intensity and height change with time. Here, the straight and collapsed pre-deformed CNTs are considered to examine the height response of the water-filled CNTs in elastic and plastic states, respectively, as shown in Fig. 2(a). The results indicate that the height of the straight water-filled CNTs is almost insensitive to but that of the collapsed water-filled CNTs increases with the electric field intensity (Fig. 2(b)). Moreover, the results in Fig. 2(c) imply that the height change of the collapsed water-filled CNTs is reversible and exhibit a rapid response to the electric field variation.

In conclusion, the simulation results reveal that the mechanical property and deformation of CNTs can be tuned through filling water molecules and applying electric field. The present research provides theoretical basis and possible design route for making nanoscale controller.

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