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Molecular Dynamics Study of Effects of Si-Doping Upon Structure and Mechanical Properties of Carbon Nanotube

SONG Hai-Yang, SUN He-Ming, and ZHANG Guo-Xiang

Department of Physics, Beijing Institute of Technology, Beijing 100081, China
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Abstract: In this paper, a Si-doped single-walled carbon nanotube (SWCNT) (7,7) and several perfect armchair SWCNTs are investigated using the classical molecular dynamics simulations method. The inter-atomic short-range interaction is represented by empirical Tersoff bond order potential. The computational results show that the axial Young's modulus of the perfect SWCNTs are in the range of 1.099 ± 0.005 TPa, which is in good agreement with the existing experimental results. From our simulation, the Si-doping decreases the Young's modulus of SWCNT, and with the increased strain levels, the effect of Si-doped layer in enhancing the local stress level increases. The Young's modulus of armchair SWCNTs are weakly affected by tube radius.

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Key words: molecular dynamics simulation, carbon nanotubes, Young's modulus, Si-doping

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