Electronic, structural, optical and pressure effects of Si_n@SWCNTs

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Abstract –In this work, we obtained well-ordered structures of Si nanowires (NWs) encapsulated in single-walled carbon nanotubes (Si_n@SWCNTs) using the molecular dynamic method (**Figure 1**). Based on these optimized structures, the structural evolution and CDF (critical deformation pressure) of Si_n@SWCNTs subjected to axial stress at 1K is also obtained. Through the analysis of pair correlation function (PCF), the density of states (DOS), and the *z*-axis polarized absorption spectra of Si_n@SWCNTs, we find that the behavior of Si_n@SWCNTs under stress strongly depends on SWCNTs' symmetry, diameter, as well as the shape of NWs, which provide valuable information on potential application in high pressure circumstance.

Si is a very important semiconductor material, so Si NWs are expected to have intriguing structural, surface, electronic, and mechanical properties. NWs composed of silicon not only have the ability to function as the device element themselves, but also offer the potential to serve as interconnects between active elements in a device. For example, Si NWs can be used to fabricate nanoelectronic devices such as nanoscale FET, nanosensors, and so on [1], and then Si NWs were gradually synthesized [2]. Some possible structures for Si NWs were theoretically predicted, their electronic and geometric structures, nanomechanics have been investigated [3]. The excellent property of Si NWs as well as the defending effect of the carbon shell suggest that Si_n@SWCNT will have tremendous application potential. The mechanical property of Si_n@SWCNT is quite important for material applications and can strongly affect the electronic or optical properties and lead to failure of the nanodevices.

In this work, all calculations were performed using the MATERIALS STUDIO molecular modeling software packages. Large-scale molecular dynamics simulations were used to study the response of Si_n@SWCNTs to an axis pressures (P_{zz}) load at 1 K. The structural evolution and CDP was obtained. Under stress applied to the whole system including both the Si NWs and CNTs, some interesting transformation take place, for example, the double parallel chains depart at the center and transform into two perpendicular parts, the string pattern transformed into helical pattern, the number of helical strand increase, helical pattern transformed into strain pattern. Especially, CDF of Si_n@SWCNTs with armchair symmetry was found higher than that with zigzag symmetry. Upon the analysis of the PCF, DOS and absorptions, we concluded that the behavior of Si_n@SWCNTs under stress strongly depends on SWCNTs' symmetry, diameter, and the shape of Si nanowires. Si_n@SWCNTs with small dimension and armchair symmetrical SWCNTs, as well as with chain structural NWs are stiffer and more difficult to collapse and with potential to apply to high pressure systems such as seabed cable.

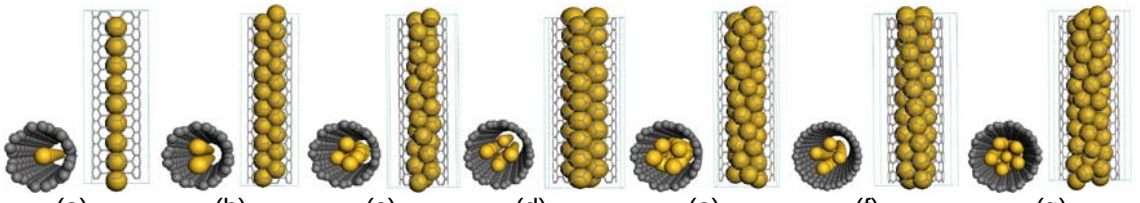

Figure 1. (Color online) Images of the Si_n@SWCNT with different diameters. (a) Si_9@(6,6)SWCNT: single atomic chain; (b) Si_{20}@(7,7)SWCNT: double chain composed of two parallel atomic chains in which the atoms are arranged in an interleaving fashion; (c) Si_{29}@(8,8)SWCNT: helical shell structure strand by three atomic strands; (d) Si_{39}@(9,9)SWCNT: four parallel single chains in which the atoms are arranged in an interleaving fashion; (e) Si_{42}@(9,9)SWCNT: helical shell structure strand by four atomic strands; (f) Si_{52}@(10,10)SWCNT: shell structure composed of four helical parallel atomic chains; (g) Si_{38}@(16,0)SWCNT: shell structure composed of five helical shell structure along with center unparallel single atomic chain; (Note: perspective snapshots with 45 degree angel show no lattice box).

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