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Energy barrier for configurational transformation of graphene nanoribbon on nanotube

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Abstract A graphene nanoribbon (GNR) has two basic configurations when winding on the outer surface of a carbon nanotube (CNT): helix and scroll. Here the transformation between the two configurations is studied utilizing molecular dynamics simulations. The energy barrier during the transformation as well as its relationship with the interfacial energy and the radius of CNT are investigated. Our work offers further insights into the formation of desirable helix/scroll of GNR winding on nanotubes or nanowires, and thus can enable novel design of potential graphene-based electronics.

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Keywords nanoscroll, helix, energy barrier, mechanics of micro/nano structures, molecular dynamics method

The graphene nanoribbons (GNRs) have potential application in future electronic devices due to their tunable band gap.[1–4] The syntheses of GNRs thus attract enormous attention.[5–8] Due to thermal fluctuations, suspended GNRs with high aspect ratio have a tendency to be in complicated grouped states,[9–11] which greatly impedes their applications. Guide the suspended GNRs into regular configurations becomes the key in mass synthesis of GNRs. Carbon nanotube-induced assembly of GNRs is one successful example to promote the thermodynamic stability of GNRs.[12–15] It has been reported that on nanotube, the winded GNRs basically have two stable configurations: helix and scroll (Figs. 1(a) and 1(e)).[12–15] For scroll, it has been reported to play important roles in innovative nano-devices such as nano-oscillator,[16] hydrogen storage,[17] water and ion tunnels,[18] and energy absorption.[19] Numerous approaches to fabricate scroll have thus been proposed,[20–23] and the assembly from GNR is the promising one.[13,14] Through static potential energy calculation, we have revealed in our previous work that the helix or scroll configuration is determined by the tube radius, bending stiffness of GNR, length of GNR, and interfacial energy.[15] However, the transformation between the two configurations remains elusive. From the views of both assembling GNR and synthesizing scroll, it is desirable to further investigate the configurational transformation of GNR on nanotube. In this letter, we have studied the transformation between the two configurations and calculated the energy barrier during the transformation with molecular dynamics (MD) simulations. Our work provides guidance for novel design of potential graphene-based nano-device.

In MD simulations, a series of zigzag carbon nanotube (CNTs) with different radius are constructed. Correspondingly the length of GNR is about $2\pi(r_0+d)+2\pi(r_0+2d)$, where r_0 is the

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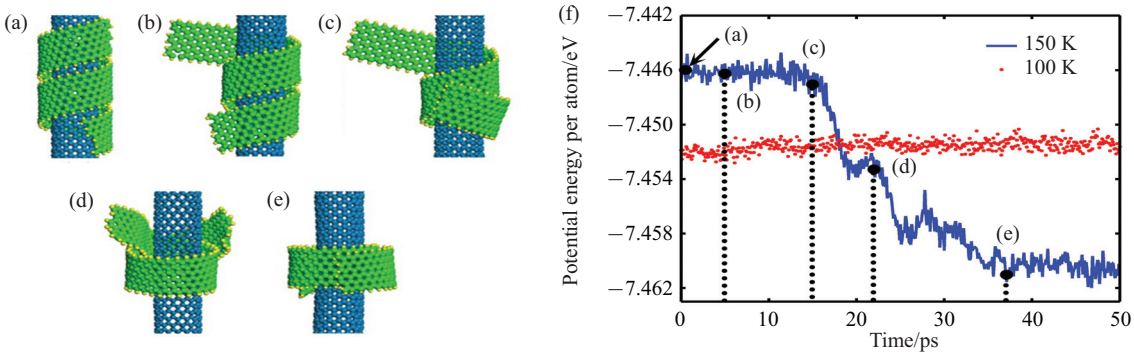

Fig. 1. Plots (a)–(e) are snapshots of transform of a GNR from helix configuration to scroll on a (14, 0) CNT. Plot (f) denotes the total potential energy per atom during this process. The solid line represents a successful transform at 150 K and the dash line for a failed process at 100 K. Labels (a)–(e) are respectively corresponding to the energy state at the time marked on plot (f).

radius of CNT and $d = 0.34$ nm the interlayer space. The width of GNR is 1.256 4 nm. All the dangling bonds in the GNR are passivated with hydrogen atoms to avoid chemical reactions. The C-C and C-H bonds are described by the adaptive intermolecular reactive empirical bond order potential (AIREBO).[24] The interaction between CNT and GNR is described by Lennard–Jones (L–J) potential $E = 4\lambda\varepsilon_{c-c}[(\sigma_{c-c}/r)^{12} - (\sigma_{c-c}/r)^{6}]$, where $\lambda = \varepsilon_{t-g}/\varepsilon_{g-g}$ is a factor tuning the intensity of the interaction,[18] ε_{t-g} is the L–J parameter between the CNT and the GNR, $\varepsilon_{g-g} = \varepsilon_{c-c} = 0.002\,84$ eV is the L–J parameter between GNR itself, and $\sigma_{c-c} = 0.34$ nm. All the MD simulations are performed using LAMMPS packages[25] with microcanonical ensemble (NVE).

To illustrate how the energy barrier prevents the helix transforming into scroll, we first set up a model system where GNR winds on a (14, 0) CNT into a helix structure (Fig. 1(a)). In our previous work we have shown that to maintain a helix structure, energetically the tuning factor λ should be a large value, otherwise the final structure would be a scroll.[15] Here we tune λ to a small one ($\lambda = 0.281$) and run a MD simulation at temperature $T = 100$ K. In a 100 ns run it is seen that the structure keeps being a helix, which is contradictory to our previous finding.[15] This contradiction could be explained by the existence of energy barrier during the transformation from helix to scroll. As we increase the temperature to 150 K, it is seen that the helix structure spontaneously transforms into scroll (Figs. 1(a)–1(e)), which means the energy barrier could be overcome via thermal undulation. The solid line in Fig. 1(f) shows the profile of potential energy of the system for the successful transformation while the dashed one represents a failed one.

Similarly, to demonstrate the existence of energy barrier within the transformation from scroll to helix, we repeat the MD simulations in which initially the GNR winds on the nanotube into a scroll (Fig. 2(a)). This time λ is set to 4.93 and according to the prediction in Ref. 15, the final configuration should be helix. However it is seen that at temperature $T = 300$ K, the configuration keeps being a scroll during a 10 ns MD run (Fig. 2(a)). The structure spontaneously transforms into the helix only when the temperature increases to 400 K. The snapshots of the process are shown in Figs. 2(a)–2(e) and the profiles of potential energy for successful and failed transformations are shown in Fig. 2(f). We conclude that the energy barriers do exist during the