Computational Materials Science 125 (2016) 146–153

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Configuration transition between graphene and nanoscroll using kinetic energy injecting method

Jiao Shi [a], Hang Yin [a], Jingzhou Yu [a], Lingnan Liu [a], Kun Cai [a,b,*]

[a] College of Water Resources and Architectural Engineering, Northwest A&F University, Yangling 712100, China
[b] Research School of Engineering, The Australian National University, ACT 2601, Australia

ARTICLE INFO

Article history:
Received 20 July 2016
Received in revised form 10 August 2016
Accepted 19 August 2016
Available online 10 September 2016

Keywords:
Nanomotor
Nanoscroll
Graphene
Carbon nanotube
Rotational kinetic energy

ABSTRACT

By placing a graphene nanoribbon (GNR) near a carbon nanotube (CNT) it is possible to obtain a carbon nanoscroll (CNS) from the GNR winding on the CNT. The original two-dimensional material, then, becomes a one-dimensional material. To shift the two types of material from the same nanocomponents, external energy ought to be injected into the CNS. Without an injecting charge or putting the system at a high temperature, rotational kinetic energy can also lead to the same result. In the present study the unwinding features of a GNR from a rotary CNT are investigated, with consideration of such essentials as the chirality of the CNT and GNR, sizes of the GNR, temperature, and defects on the CNT. The driving power of the CNT for unwinding the GNR depends on the interaction between the two components. Some remarkable conclusions are drawn which are helpful in potential applications of the geometry shifting of the CNS.

1. Introduction

As a peculiar two-dimensional (2D) nanomaterial, graphene [1] has attracted much attention from researchers and scientists in recent years. It is well known that graphene has excellent mechanical properties due to in-plane sp^2-sp^2 covalent bonds [2] and electrical properties due to delocalized electron (π electron) on each carbon atom [3]. By virtue of these excellent physical properties, graphene is an important candidate material for use in the next generation of nano-electro-mechanical systems [4]. It is difficult to maintain a piece of graphene nanoribbon (GNR) [5] in its original configuration, i.e., a plate sheet, when it leaves a substrate. When the in-plane size of a GNR is far greater than its thickness of ~0.34 nm, it rapidly changes into a nanofolder [6] or nanoscroll [7] to reduce surface potential energy. One method for forming a scroll rather than a folder from a GNR is to put a carbon nanotube (CNT) [8–10] or a nanowire near one side of the GNR [11,12]. The carbon nanoscroll (CNS) obtained from winding of a GNR has two open axial boundaries: an inner boundary and an outer boundary, unlike a CNT that has an enclosed boundary. Hence, the radius of the scroll is adjustable, which is essential to applications of hydrogen storage [13], mass transport [14], and high capacity lithium ion batteries [15]. In recent years, the properties of graphene structures have been investigated both experimentally [16–18] and by numerical simulation [19–21]. Using experiments, Yan et al. [15] achieved a CNS by self-assembly of graphene on a nanowire with length over 30 μm. Zhang and Li [16] built an oscillator from a GNR on a CNT, and studied the oscillation characteristics of the CNS with/without bridged edges. Perim et al. [12] suggested a method of forming a CNS from a nanoribbon and a CNT: when the CNT is placed on one end of a graphene sheet which is simply supported by a substrate, the nanoribbon will scroll rapidly onto the CNT. Using density functional theory (DFT)- based calculation, Sorkin and Su [17] found the phase transformation from diamond nanowires to other nanostructures including CNS at high temperature. Recently, researchers have also suggested hydrogenation methods to fold or scroll a GNR [18]. The mechanisms are such that the graphene curves at the hydrogenated area, and when the curvature is high enough to trigger the graphene to reduce its surface itself, the CNS forms rapidly to reduce the surface potential energy. For example, Liu et al. [19] used C_4H-type of graphene to form a CNS by itself or by scrolling onto a CNT. Reddy and Zhang [20] investigated the relationship between the curvature and the layout of the hydrogenated area. Zhu and Li [21] used such a method to form a nanocage from hydrogenated graphene after tailing it with desired shapes.

As the GNR is scrolled, the original 2D material becomes a one-dimensional (1D) material, a phenomenon that implies that some physical properties such as electrical and thermal conductivity undergo significant change. If we need the properties of both 2D and 1D nanomaterials to vary one after the other, in turn, the CNS

* Corresponding author at: College of Water Resources and Architectural Engineering, Northwest A&F University, Yangling 712100, China.
E-mail address: kun.cai@anue.edu.au (K. Cai).

http://dx.doi.org/10.1016/j.commatsci.2016.08.025
0927-0256/

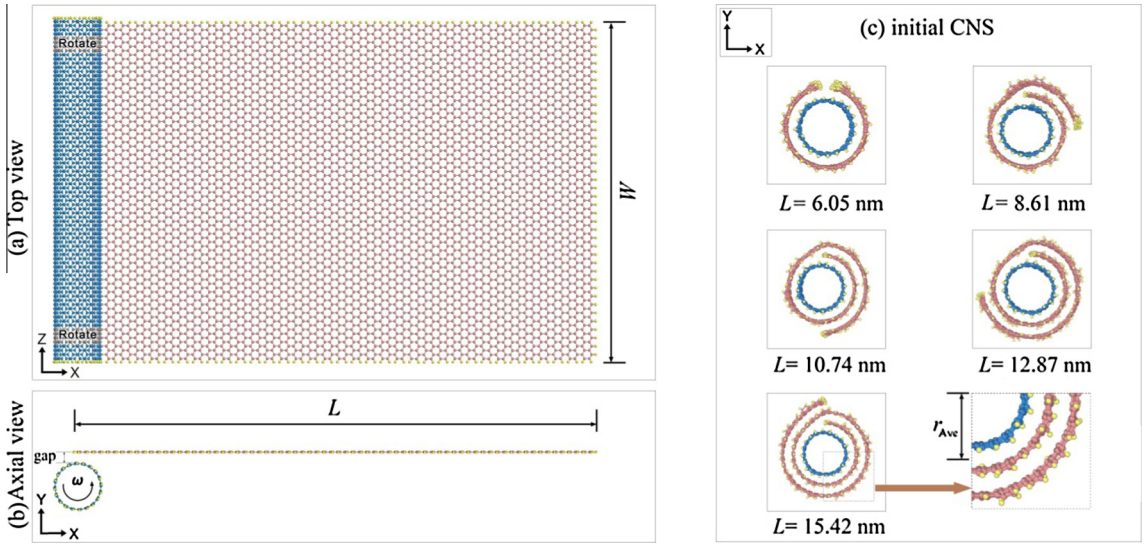

Fig. 1. Initial models of a CNT over a GNR. Each carbon atom on the edges of a tube or GNR is bonded with a hydrogen atom. (a) Top view of the model before forming a CNS. (b) Axial view of the model. Here the rotational direction of the CNT is **anticlockwise** with the frequency of ω after forming a stable CNS. The initial value of the "gap" between the CNT and the GNR is 0.34 nm. The length of the CNT is ~10 nm. The length and width of the GNR are L and W, respectively. (c) At the initial equilibrium state of the CNS, the length L of GNR is assumed to be 6.05, 8.61, 10.74, 12.87, and 15.42 nm, respectively. The GNR winds clockwise onto the CNT (from inner to outer). "r_{Ave}" is the average radius of the CNT and the adjacent curved GNR. In the model shown in (a), the axial length of the tube is identical to W, i.e., the width of the GNR. In simulation, except for considering the effect of the width of the GNR, W is set to be 10 nm. In (a), (10,10) CNT and armchair type GNR are adopted. The type of GNR is defined by the configuration of the level sides of the GNR. In the present simulation, four types of CNS are considered, and the related parameters are listed in Table 1.

should be unwound. As an inverse process, when a CNS is unwound into a 2D material, external energy would be put into the scroll. Typically, three methods can provide the energy to unwind the scroll. The first method injects charge into the scroll [22]. As soon as the electric potential energy is high enough, the CNS becomes a plate that contains lower potential than a scroll. Shi et al. [23] even controlled the rolling/unrolling of a CNS on a rigid substrate via an external electric field. The second method is a thermal method. For example, Yi et al. [24] suggested a method of unwinding a nanoscroll or nanofolder into a planar ribbon by adjusting the ambient temperature. Besides these two methods, we can also release a CNS by introducing kinetic energy on it. In present work, a GNR that has been wound onto a CNT would be released from the CNT with high rotational frequency [25–27]. Many factors, related either to the system parameters or to the environment, are essential to the releasing process of CNS. To develop comprehensive understanding of the rotation-based unwinding, more features of unwinding are investigated in the present work. Such factors as the chirality of the CNT, the in-plane size of the GNR, defects on the CNT, and the environmental temperature are considered in our molecular dynamics (MD) simulations.

2. Model and method

For the sake of simplicity, the (10,10) CNT is labeled A-CNT and the (17,0) CNT is Z-CNT. The armchair GNR is labeled A-GNR and the zigzag GNR is Z-GNR.

The major steps in each simulation task are as following. Step (1) Build the model. Step (2) Minimize the potential energy of system, as shown in Fig. 1a, using the steepest descent algorithm with the tolerances for energy and force of 10^{-4} and 10^{-6}, respectively. Step (3) Initiate the velocities of atoms in the box with the temperature of 300 K. Step (4) Actuate the rotation of the CNT by applying a rotational period on the gray areas on the tube, e.g., 5 ps (or 200 GHz) in the present study, and put the system in a canonical NVT ensemble with the temperature of the rest of the CNT and the GNR to be 300 K, separately. Step (5) Run and collect data for post-processing. The simulation stops after the GNR is entirely unwound from the CNT.

The open-source code LAMMPS [28] is adopted for the present simulations. The AIREBO [29] potential is used to describe the force field of the carbon-hydrogen system. The time step for updating of the positions and velocities of atoms is 1 fs.

3. Results and discussion

3.1. Effect of chirality pairs of tube and GNR

As the interaction between CNT and GNR is sensitive to their chirality, this difference is discussed first. For convenience in discussion of the process of winding/unwinding of GNR between plate and scroll, the variations of potential energy (VPE) of CNT and GNR are defined as

$$\begin{cases} \Delta E_{CNT} = E_{CNT,Sys} - E_{CNT} \\ \Delta E_{GNR} = E_{GNR,Sys} - E_{GNR} \end{cases} \quad (1)$$

where $E_{CNT,Sys}$ is the potential energy of the CNT in the system (Fig. 1c). That is different from the potential energy of a pure CNT (E_{CNT}). $E_{GNR,Sys}$ is the potential energy of the curved GNR in the system and E_{GNR} is the potential energy of the curved GNR without a CNT nearby.

When the CNT is rotating, the GNR is driven to rotate due to friction between the CNT and the GNR. The rotational kinetic energy (RKE) of the GNR can be obtained using the equation:

$$K_{GNR,Rotat} = K_{Sys} - K_{CNT} - K_{GNR,Therm} \quad (2)$$

where K_{Sys} is the total kinetic energy of system, K_{CNT} is the total kinetic energy of the CNT, and $K_{GNR,Therm}$ is the kinetic energy with respect to the thermal vibration of atoms, determined by the number of atoms on the GNR and the temperature.

The solid blue[1] curves in Fig. 2 show the VPE histories of the CNTs during winding of the GNRs onto them, for the four models listed in

[1] For interpretation of color in Fig. 2, the reader is referred to the web version of this article.