Formation of Single Walled Carbon Nanotube Via the Interaction of Graphene Nanoribbons: Molecular Dynamics Simulation

A. J. Du*,**, Sean C. Smith *,** and G. Q. Lu**
*Centre for Computational Molecular Science, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, QLD 4072, Brisbane, Australia, a.du@uq.edu.au and s.smith@uq.edu.au
**ARC Centre for Functional Nanomaterials, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, QLD 4072, Brisbane, Australia, maxlu@cheque.uq.edu.au

ABSTRACT

Classical Molecular Dynamics simulations were carried out to study the interaction of two zigzag graphene nanoribbons (GNRs). Remarkably, single walled armchair carbon nanotube could be formed via two zigzag GNRs at room temperature. The reaction process strongly depends on the distances between two ZGNRs and the widths of ZGNR. Our results suggest an effective route for the controllable growth of specific armchair nanotube.

Keywords: Graphene Nanoribbon, Single walled carbon nanotube, Molecular Dynamics

1 INTRODUCTION

Since the discovery of fullerenes and carbon nanotubes, low-dimensional nanoscale carbon materials has been the subject of intensive research during the past two decades due to the peculiar electronic structures that are expected to be important for practical applications in nanoelectronics [1-2]. Recently, single graphite layers, referred to as Graphene nanoribbons (GNR) have been prepared experimentally by using conventional device set up [3-4]. Such findings have opened up exciting opportunities for the design of novel electronic devices and interconnects, e.g., quantum information processing [5] and tiny transistors [4, 6]. Theoretically, the energy gaps and optical properties have been predicted with various widths by Son et al. and Barone et al [7-8], respectively. These provided a qualitative way of determining the electronic properties of ribbons with widths of practical significance. More recently, results obtained in the Berkeley lab show that zigzag graphene nanoribbons are magnetic and can carry a spin current response to the external electric field. This opens a new path to the application of spintronics [9].

Generally, SWCNTs are typically grown as mixtures of metallic and semiconducting tubes, depending on the arrangement of the hexagonal rings along the tubular surface [10]. However, this actually constitutes one of the notable obstacles to the widespread application of this unique material, since metallic and semiconducting materials have very different functions in nano-devices. Hence, separating them has become a central issue in terms of effective fabrication of high performance electronic devices. Currently, many physical and chemical methods have been developed for the separation according to the respective electronic properties by using dielectrophoresis [11-12], selective flocculation [13], selective adsorption of the functional group [14-15], and density gradient induced centrifugation [16] so on. However, none of these is satisfactory from the point of view of high throughput, better selectivity and yield, and more favorable scalability [17].

Bare GNR also has unsaturated dangling bonds at zigzag. Clearly a single graphene sheet is very difficult to roll into a SWCNT without any catalyst. An intriguing question, however, is whether it is possible to form SWCNT via the interaction of bare ZGNRs? To explore this question, we report below a molecular dynamics (MD) simulation to study the interaction of bare GNRs with zigzag shaped edges. We found that two bare nanoribbons (N_z=8) with zigzag shaped edge could form a (8, 8) single-wall armchair carbon nanotube at room temperature, suggesting a possible route for selective synthesis and growth of armchiair nanotubes via the interaction of ZGNRs.

2 COMPUTATIONAL DETAILS

MD simulation was performed by putting two 8-ZGNRs at natural separation distance of graphite layers (3.3 Å). The second-generation reactive empirical bond order potential (REBO) developed by Brenner was used to describe the C-C and C-H interaction [18]. Long distance van der Waals forces expressed in 6-12 Lennard-Jones form were also taken into account. The simulated system contains 1600 Carbon and 32 H atoms. Temperature was controlled by Langevin scheme at room temperature.

3 RESULTS AND DISCUSSION

ZGNRs are classified by the number of zigzag chains (N_z) across the ribbon width as shown in Fig 1. 8-ZGNR represent GNR with 8 zigzag chains. First, geometry optimization for 8-ZGNR with and without H-termination were performed utilising the conjugate gradient method.

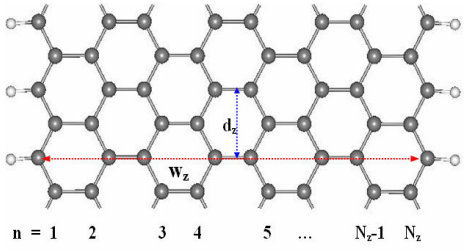

Figure 1 Geometry structure for hydrogen terminated graphene nanoribbons (GNRs) with zigzag shaped edges. The grey and white balls represent C and H atoms, respectively. The 1D unit cell distance and the ribbon width are denoted by d_z(Wz) for 8-ZGNR.

Apparently, the existence of dangling carbon bonds in the bared GNR should offer a much higher chemical reactivity to manipulate the interaction of ZGNRs. Here we performed MD simulation at 300K for two 8-ZGNRs positioned at a distance of 3.3 Å, which is very close to the natural separation of two graphite layers. Our MD simulation was based on the canonical (NVT) ensemble. Figure 2 present the energy profile along the MD trajectory. It can be seen that a (8,8) armchair SWCNT was formed around 160 ps.

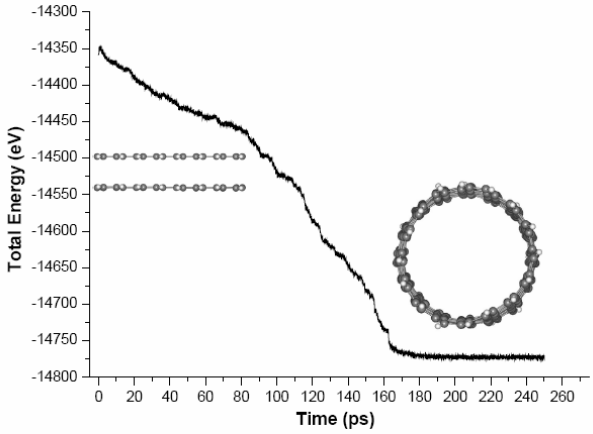

Figure 2 the variation of total energy along MD trajectory for the interaction of two 8-ZGNRs.

Then we turn to study the effect of the distance between two 8-ZGNRs. Two distances, 3.2 and 5.0 Å were set for two separated MD run. Figure 3a present their energy profiles along the MD trajectory. Width could be also very important during the formation of SWCNT via the interaction of ZGNRs. Here we performed another two MD runs at different ribbon widths, i.e. 6-ZGNR and 18 ZGNR. The energy profile along MD trajectory was presented in Figure 3b. Clearly, the formation of SWCNT is faster when distance between two 8-ZGNRs is short (3.2 Å) and the width of ZGNR is narrow (6-ZGNR).

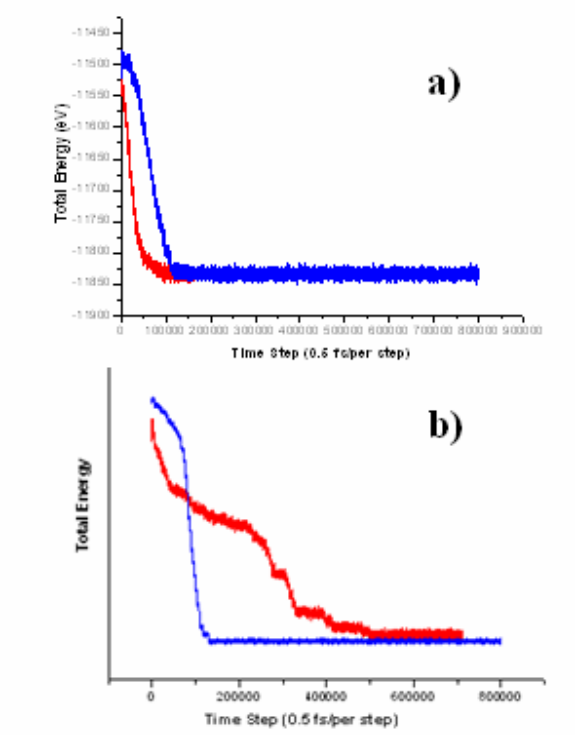

Figure 3 a) Energy profiles along the MD trajectory for the distance of two ZGNRs are 3.2 (red) and 5.0 Å (blue), respectively. b) for the 6-ZGNR (blue) and 18-ZGNR (red), respectively

In order to build reliable microelectronic nano-devices based on SWCNTs, selective processes must be developed to create SWCNTs with specific electronic and mechanical properties. Despite many experimental efforts directed towards the separation of metallic and semiconducting nanotubes, most of them are actually not selective for the diameter and chirality [19]. Furthermore, techniques such as chemical functionalization may also introduce defects and require further processing to restore the useful electronic properties of SWCNT. Hence, improved techniques are still needed. More recently, Smalley's group has developed a cloning method to cut up individual nanotubes into short segments that act as the seeds for regrowing entire tubes [20]. In light of exciting recent progress on the controllable growth of two dimensional GNRs with various widths, these results suggest an alternative approach to the selective synthesis of SWCNTs with specific diameter and chiarility that may provide an interesting avenue for future investigations.

4 CONCLUSIONS

In summary, the interactions of two bare 8-ZGNRs with were investigated by *a classical Molecular Dyanmics based on the*

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Brenner potential. Remarkably, two bare 8-ZGNRs could form a (8, 8) armchair SWCNT even at room temperature. Additionally, the interaction also strongly depends on the distance and width of ZGNRs. Considering the challenges in separating metallic and semiconducting SWCNT experimentally, our results suggest a possible alternative route to selectively synthesize specific types of nanotubes via GNRs.

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