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Formation of core-shell structure from carbon nanotube and silver nanowire

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ABSTRACT

In recent year, carbon materials have attracted an intensive interest for scientists to propel the development of nanotechnology. In this manuscript, using forced-field-based molecular dynamics simulations, the interaction between the carbon nanotubes (CNTs) and silver (Ag) nanowires (NWs) has been investigated. The results show that the Ag NW can induce the self-assembly of the CNTs to form a shell-core structure, and the van der Waals interaction and the offset face-to-face π-π stacking interaction play an important role in this process. Furthermore, the size (diameter) of the CNTs should meet some required conditions to guarantee the shell-core configuration and different surface of Ag NWs exhibits different result. Moreover, different metal nanowires were also discussed.

1. Introduction

Recently, Carbon nanotubes (CNTs) who own hollow cylindrical structures made of networks of carbon atoms, have exhibited outstanding thermal conductivity, electrical properties and mechanical strength [1]. These significant properties have attracted great attention for scientists to explore their potential applications in nanosized electronical and mechanical devices, especially for the fabrication of CNTs composites [2,3]. The functional CNTs composites have caught researchers' great imaginations due to the broad prospects in sensors, hydrogen storage, nanodevices, electromagnetic wave absorption, heterogeneous catalysis, as well as biomolecular and drug delivery in the field of biology [4–6]. The CNTs composites can be fabricated through the encapsulation of foreign fillers in the CNTs or the wrapping of polymers around the outside or inside wall of the CNTs [7–10]. In a general way, the idealized cylindrical geometry of CNTs deform and change to various cross-sectional shapes, such as oval, trigon, peanut and ribbon shapes, due to the van der Waals interaction 13 between CNTs and the substrate. Moreover, both theoretical and experimental results demonstrated that the CNTs' superior properties can be affected by the deformation and defects of the CNTs [11,12].

Wei et al. [13] reported that Al nanowires (NWs) can activate, guide and stabilize the self-assembly of the CNR to form a double-deck helix, as a result of the combined action of the van der Waals interaction and the offset face-to-face p–p stacking interaction. Yan and his coworkers [14] reported the radical collapse and self-scroll of the CNTs induced by Cu NWs, resulting in the coaxial core–shell composite nanostructure. This composite not only greatly change the properties of the pristine tube, but also protect the inner NW against oxidation and shape fragmentation. This result inspires us to imagine how the super-short carbon nanorings and NWs interact. The super-short carbon nanorings can also be regarded as enclosed and rolled narrow graphene nanoribbons (GNRs) [15,16]. The CNRs with a large diameter tend to be thermodynamically unstable and collapse, which makes the wrapping of the CNRs around the NWs [17,18].

In this study, using molecular dynamics simulations, the interaction between CNTs and Ag NWs is revealed and the final shape of the CNTs adhering to the Ag NWs is also discussed. In addition, many complicated factors are also dispalyed which may influence the final configuration of the CNTs. This work is not only significant to the better understanding of the self-assembling process but also vital for the fabrication of novel CNTs-based composite structures. In this paper, we just simulated the physical interaction between the CNTs and NWs, dominated by the van der Waals interaction, without considering the chemical bonding. An exhaustive follow-up study is also needed to clarify the chemical interactions.

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2. Computational methods

In this work, the atomistic interaction is described by the force field of condensed-phase optimized molecular potentials for atomistic simulation studies (COMPASS) [19]. It is an *ab initio* force field that has been parametrized and validated using condensed-phase properties in addition to various *ab initio* calculations and experimental data. It has been proven to be applicable in the prediction of properties of CNTs [13,20]. The molecular dynamics simulations are carried out under a constant volume and constant temperature (NVT) ensemble with a temperature of 298 K. The Nose method in the thermostat is employed to control the thermodynamic temperature, which can be kept constant by allowing the system to exchange energy with a"heating bath", and generate the correct statistical ensemble. The time step is chosen to be 1.0 fs, and data are collected at intervals of 2.0 ps. Then the full-precision trajectory is recorded for further analysis. Herein, we prepared the simulation models consisting of the Ag NWs and CNTs. All Ag NWs are fixed as rigid structures, the axes of which are positioned in the (111) direction. Initially, all CNTs are placed in the middle of the Ag NWs, with the separation of 5 Å. Each of the CNT-NW system is sufficiently relaxed to achieve an equilibrium state.

3. Results and discussion

3.1. The formation of Ag-carbon nanoscoll core-shell structure

The formation of Ag-carbon nanoscoll(CNS) core-shell NWs is simulated by the molecular dynamic (MD) method. Fig. 1 shows some snapshots of the interaction between the CNT (60, 60) with 81.36 Å diameter and 28.3 Å diameter Ag NW from 0 to 50 ps, respectively. It can be seen that the formation process has two steps. Firstly, the CNT collapses, and then CNT scrolls around the Ag NW. At the beginning, the CNR with a diameter of 81.36 Å tends to be thermodynamically unstable, resulting in discontinuous ripples and wrinkles in the circumference [21]. With the simulation time going on, due to the strong attraction force, the CNT and the Ag NW approach to each other. And then the surface of the CNT which is closer to the Ag NW moves rather faster because carbon atoms closer to Ag NW endure stronger van der Waals force. Therefore, CNT (60, 60) deforms as a peach along the approaching direction as shown in 1 ps snapshot in Fig. 1. When the simulation time reaches to 10 ps, the opposite walls of the CNT are close to each other, and collapse into a cucurbit shape on the Ag NW. With the simulation time going on, the cucurbit shape continues to change to long bean (20 ps), hook (30 ps, 40 ps). Then, CNT experiences successive collapse to form a carbon nanoscroll. Simultaneously, the axes of the CNR and Ag NW begin to offset and the flattened nanoribbon shows a double-walled graphitic nanoribbon around the Ag NW with a certain pitch. At 48 ps shown in Fig. 1, when some of the top and bottom atoms of CNT get close enough to each other, the collapse is further accelerated due to the π-π stack effect between the top layer and bottom layer of the collapsed CNT and then the core-shell (Ag-CNS) nanostructures are produced eventually.

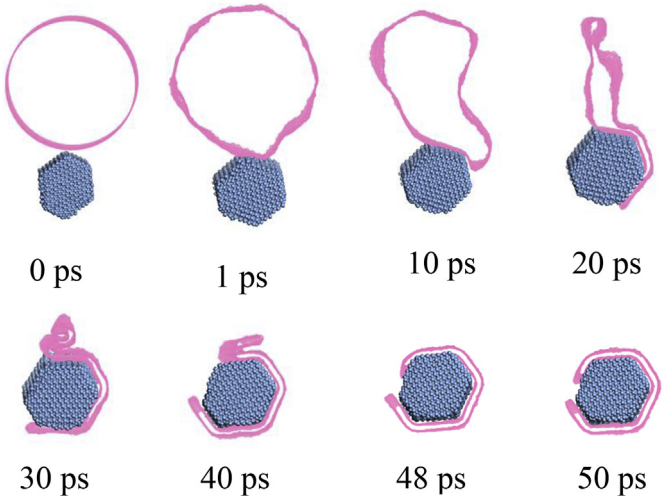

Fig. 1. Typical snapshots of collapse of the CNT (60, 60) with a diameter of 81.36 Å on the Ag NW with the diameter of 28.3 Å. The length of the Ag NW is 113.2 Å and that of the CNT is 36.89 Å.

3.2. The mechanism of the formation of the core-shell structure

In order to reveal the formation process of the core-shell structure, we plot the curves of the total potential energy (Ep) in Fig. 2. From the Fig. 2, it can be seen that the total potential energy shows a significant decreasing during the first 48 ps, suggesting that both the collapse and core-shell formation processes are spontaneous. As we known, the lower the energy, the much more stable states. Due to the obvious decreasing energy, these two CNT-NW systems increase contact areas and gradually reach more stable states. Finally, after 50 ps, the energy reaches its minimum and subsequently remains at the minimum value with some minor fluctuations, indicating that the whole system reaches its equilibrium.

The geometric characteristics of the CNT-NW system can be indicated by the concentration distribution profiles. Fig. 3 shows the concentration profiles of the core-shell composite structure in the X and Y directions. Furthermore, the peaks which are depicted in details are also labeled in Fig. 3. From Fig. 3, it can be seen that the distance between the NW and the CNR layer is about 3.0 Å, which is very close to the scale of the chemical bonding. This shorter distance indicates that the interaction between the collapsed CNT and the NW is very strong. Moreover, the separation between the two layers of the collapsed graphene nanoribbon is exactly close to 3.5 Å, which is in good agreement with the wall thickness of the multiwall CNTs (3.4 Å) and also in accordance with the parallel stacking distance of the offset face-to-face π-π stacking interactions.

From mentioned above, it is urgent to known how the CNR spontaneously collapses on the Ag NW and sticks on the NW. In

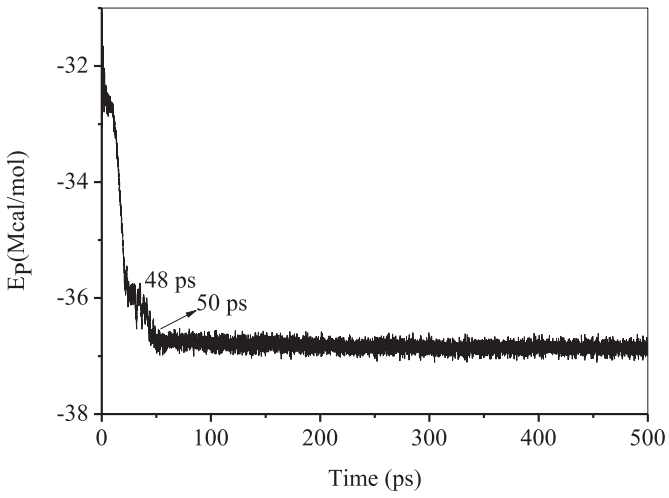

Fig. 2. Total potential energy (Ep) of the CNT-NW system as a function of time.