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Buckling instability of carbon nanoscrolls

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Formed by rolling up a monolayer graphene into a spiral structure, a carbon nanoscroll (CNS) is topologically open and has two free edges along its axial direction, distinct from a multi-walled carbon nanotube (MWCNT). Through systematic molecular mechanics simulations, we show that the unique structure of a CNS produces distinct features of its buckling instability under axial compression, twisting, and bending from those of a MWCNT. The results should be instrumental in future structural design of CNS-based applications. As an example, we demonstrate molecular mass transport through a CNS enabled by its torsional buckling instability. The understanding of reversible buckling instability of CNSs could potentially enable the design of novel nano-devices. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4754312]

I. INTRODUCTION

The observation of scrolled packets of graphite plates under surface rubbing was first reported in 1962.¹ Significant progress on fabricating high-quality monolayer graphene in last several years² has led to surging interests in scrolled graphene at nanoscale.^{3–6} A carbon nanoscroll (CNS) is formed by rolling up a monolayer graphene into a spiral multilayer nanostructure (Fig. 1(a)). A CNS is topologically open (for example, the core size of a CNS is highly tunable by relative sliding between adjacent layers).⁴ By contrast, a CNT is topologically closed, thus its core size can only be changed slightly by stretching the carbon-carbon (C-C) bonds. The topologically open and highly tunable structure of CNSs, together with the exceptional mechanical and electronic properties inherited from the basal graphene, has inspired an array of novel nano-device applications, such as hydrogen storage medium,^{7,8} water and ion channels,⁹ and ultra-fast nano-oscillators.^{10,11} Meanwhile, the topologically open structure of CNSs along with the large out-of-plane flexibility of its one-atom thick basal graphene suggests the proneness of CNSs to buckling instability under mechanical loads. Buckling instability of a CNS not only substantially reduces its structural rigidity but also causes significant changes in its electronic and magnetic properties.¹² The success of CNS-based device applications crucially hinges upon systematic understanding of the buckling instability of CNSs under various mechanical loads, a topic that remains largely unexplored.

Buckling instability of CNTs has been extensively studied in recent years.^{13–21} Results from analytic models and numerical simulations have shown that CNTs are susceptible to various buckling instability under axial compression, bending, and torsion. Buckling of CNTs under bending is also observed in experiments.²² However, the fundamental difference in the topology of a CNS and a multi-walled carbon nanotube (MWCNT) leads to their dissimilar deformation behaviors under mechanical loads, and thus produces distinct characteristics of the buckling instability of the CNS from that of the MWCNT. For example, a CNS is intrinsically a one-layer spiral structure (Fig. 1(a)). Therefore, a local displacement perturbation in a CNS may propagate through the strong C-C covalent bonds in the basal graphene and thus impact the overall deformation behavior of the CNS. In a MWCNT, however, local deformation in one carbon cube only interacts with neighboring concentric carbon tubes via rather weak van der Waals (vdW) forces (Fig. 1(b)). Another distinct structural feature of a CNS that is absent in a MWCNT is the two free edges in axial direction (one along inner core and another along outer surface). These free edges are subject to intrinsic compressive edge stress and tend to wrinkle at equilibrium state (inset in Fig. 1(a), similar to the wrinkled free edges in graphene.²³ The intrinsic wrinkles along the free edges serve as geometric perturbations that could initiate deformation instability of CNSs under mechanical loads. The above distinct features of



FIG. 1. The perspective and cross-section views of (a) a 4-layer CNS and (b) a 4-layer MWCNT, respectively. The inset in (a) shows the intrinsic wrinkles along the outer free edge of the CNS at equilibrium. Similar wrinkles exist along the inner free edge of the CNS.

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CNSs are expected to have strong effects on the buckling instability of CNSs, which cannot be fully described by the existing understanding of buckling instability of CNTs.

We report a systematic study of the buckling instability of CNSs under axial compression, torsion, and bending, using molecular mechanics simulations. Particular efforts are placed on clarifying the difference in the critical buckling conditions between CNSs and MWCNTs. We find that, under axial compression, the critical buckling onset strain of a CNS with various diameters (i.e., number of layers) remains nearly a constant. By contrast, that of a MWCNT depends strongly on its diameter. Under torsion, the critical buckling onset twisting angle of a CNS is much lower than that of a MWCNT of similar diameter and only slightly higher than that of a single-walled CNT (SWCNT) of similar diameter. Under bending, the critical buckling onset curvature of a CNS and that of a MWCNT of similar diameter is comparable, due to rather localized buckling deformation. The results should be instrumental in future structural design of CNS-based applications. The understanding of tunable and reversible morphologic instability of CNSs could also potentially enable the design of novel nano-devices.

II. COMPUTATIONAL MODEL

The CNSs in the simulations in Sec. III have a length of 20 nm and diameters from 2 nm to 6 nm depending on the number of layers, with its spiral ends being armchair. The inner radius of CNSs is 0.8 nm. As a comparison with an *n*-layer CNS, an *n*-layer MWCNT with the same length is also modeled. The chirality of the *n*-layer MWCNTs is indexed by (10/10)@(15/15)@...@(5(n + 1)/5(n + 1)). The MWCNTs are carefully chosen to ensure that they have approximately same numbers of carbon atoms as their corresponding CNSs. The cross-sections of a 4-layer CNS and a

4-layer MWCNT are shown in Fig. 1. The second-generation reactive empirical bond order potential²⁴ and 12-6 Lennard-Jones potential²⁵ are adopted to describe the C-C covalent interaction and vdW force, respectively. Large-scale atomic/molecular massively parallel simulator (LAMMPS) is used in all the simulations.²⁶ During the simulation, loading is applied onto the structures incrementally and the potential energy is minimized between two loading increments. Energy minimization is conducted using a conjugate gradient algorithm, followed by a Hessian-free truncated Newton algorithm, until either the total energy magnitude is less than or equal to 10^{-15} or the total force is less than 10^{-5} eV/Å.

III. RESULTS AND DISCUSSION

A. Buckling under axial compression

To apply axial compression onto a vertically aligned CNS (or a MWCNT), five bottom rows of carbon atoms are fixed and five top rows of carbon atoms are moved downward 0.01 nm in each loading increment. In each loading increment, other carbon atoms in between are also moved downward with a displacement linearly proportional to the distance between the atom and the bottom of the CNS (or the MWCNT). This loading algorithm reduces the minimization time and avoids local instability near the two ends of the CNS (or the MWCNT).

Figure 2(a) plots the axial force vs. applied strain curves of a 4-layer CNS and a 4-layer MWCNT under axial compression, respectively. Before the onset of buckling, the slopes of the two curves are nearly identical, indicating comparable in-plane stiffness of the CNS and the MWCNT along axial direction. The cross-section topology has little impact on the pre-buckling axial stiffness of the CNS and the MWCNT. The sharp drop of the axial force in each curve



FIG. 2. (a) Axial force as a function of axial compressive strain for a 4-layer CNS (solid line) and a 4-layer MWCNT (dashed line), respectively. Insets ① and 2 show the deformed shapes of the 4layer MWCNT at a strain of 3.2% (right after onset of buckling) and a postbuckling strain of 4.9%, respectively. Insets 3 and 4 show the deformed shapes of the 4-layer CNS at a strain of 2.5% (right after onset of buckling) and a postbuckling strain of 4.2%, respectively. Color shades represent levels of potential energy. (b) Axial force as a function of axial compressive strain for CNSs (solid lines) and MWCNTs (dashed lines) of various diameters (2 to 7 layers). (c) Critical buckling onset strains ε_{cr} of a MWCNT, a CNS, and a SWCNT as a function of their diameter, respectively. The solid line without label plots a theoretical prediction for the SWCNT case (i.e., Eq. (3) in Ref. 13).

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indicates the onset of buckling. While the 4-layer MWCNT buckles at a critical axial compressive strain of $\varepsilon_{cr} = 3.2\%$, the 4-layer CNS buckles at a much smaller $\varepsilon_{\rm cr} = 2.5\%$. The snapshots of the 4-layer MWCNT and the 4-layer CNS right after buckling onset are shown in insets ① and ③ in Fig. 2(a), respectively. Both CNS and MWCNT exhibit tube buckling profile rather than beam buckling profile, given the relative small aspect ratio of the simulation models. At the onset of buckling, the 4-layer MWCNT has three symmetric folds along the length direction, while the 4-layer CNS only has two folds, possibly because the CNS buckles at a lower strain level and the strain energy released upon buckling is insufficient to form three folds. Further loading leads to the formation of the third fold in the 4-layer CNS, as indicated by the second (less significant) drop of the axial force in the corresponding curve in Fig. 2(a). The deformed shape of the CNS at post-buckling becomes similar to that of the MWCNT (insets ④ and ② in Fig. 2(a), respectively), except for the bulging out of its outer free edge.

Figure 2(b) further plots the axial force vs. applied strain curves of CNSs and MWCNTs with various diameters (2 to 7 layers) under axial compression. The pre-buckling axial stiffness of a CNS is comparable to that of the MWCNT with the same number of layers; the critical buckling onset strain ε_{cr} of a CNS is much smaller than that of its counterpart MWCNT. Figure 2(c) plots ε_{cr} of CNS and MWCNT as a function of their diameter, respectively. ε_{cr} of a MWCNT decreases significantly as its diameter increases. Interestingly by contrast, ε_{cr} of a CNS remains approximately a constant, nearly independent on its diameter. Such a distinction in buckling behavior can be explained as follows. For a MWCNT, its outermost tube is most prone to compressive buckling. Once it buckles, its unsymmetrical radial deformation perturbs the inner tubes via vdW interactions and leads to the overall buckling of the MWCNT. Although the existence of inner tubes helps stabilize the deformation of the outermost tube in MWCNTs, the critical buckling onset strain of a MWCNT is largely dictated by its outermost tube. That is, its ε_{cr} decreases as its diameter increases. The above argument is supported by the further simulation results of $\varepsilon_{\rm cr}$ of SWCNT as a function of its diameter, which is in agreement with Yakobson's theoretical prediction¹³ that ε_{cr} of a SWCNT under compression is inversely proportional to its diameter (as shown in Fig. 2(c)). For a CNS, however, the wrinkles along its free edges (especially the outer free edge that is less constrained) are highly vulnerable to further buckling under compression (e.g., inset ③ in Fig. 2(a)), which can further propagate along the spiral basal graphene through C-C covalent bonds, resulting in the overall buckling of the CNS. In other words, ε_{cr} of a CNS under compression is largely dictated by the intrinsic fluctuations along its free edges, thus is nearly independent on its diameter.

B. Buckling under torsion

Torsion is applied onto a vertically aligned CNS (or a MWCNT) by fixing the five bottom rows of carbon atoms and rotating five top rows of carbon atoms in counterclockwise direction by 1° in each loading increment. Similar to the loading algorithm used in compression, other atoms are also rotated by an angle proportional to their distance from the bottom end.

Figure 3(a) plots the resultant torque as a function of twisting angle per unit length for a 4-layer CNS and a 4-layer MWCNT, respectively. The distinction between the CNS and the MWCNT under torsion is threefold. First, the CNS has much smaller torsion rigidity than the MWCNT before buckling onset, indicated by initial slope of the two curves. Second, the critical buckling onset twisting angle θ_{cr} for the CNS is much smaller than that of the MWCNT. For



FIG. 3. (a) Resultant torque as a function of twisting angle per unit length for a 4layer CNS (solid line) and a 4-layer MWCNT (dashed line), respectively. Insets ① and ② show the deformed shapes of the 4-layer MWCNT at a twisting angle of 0.049 nm^{-1} (right after onset of buckling) and a postbuckling twisting angle of 0.07 nm⁻¹, respectively. Insets 3 and 4 show the deformed shapes of the 4-layer CNS at a twisting angle of 0.021 nm⁻¹ (right after onset of buckling) and a postbuckling twisting angle of 0.041 nm^{-1} , respectively. Color shades represent levels of potential energy. (b) Resultant torque as a function of twisting angle per unit length for CNSs (solid lines) and MWCNTs (dashed lines) of various diameters (2 to 5 layers). (c) Critical buckling onset twisting angle $\theta_{\rm cr}$ of a MWCNT, a CNS, and a SWCNT as a function of their diameter, respectively.

example, $\theta_{cr} = 0.047 \text{ nm}^{-1}$ for the 4-layer MWCNT, and 0.020 nm^{-1} for the 4-layer CNS. As a result, the CNS upon the onset of twist buckling has a less distorted profile than that of the MWCNT (insets 1) and 3 in Fig. 3(a)). Third, the drop in resultant torque for the 4-layer CNS at the onset of buckling is much smaller and less sharp than that for the 4layer MWCNT. These distinctions in the deformation behavior of the CNS from that of the MWCNT can be largely attributed to the open topology of CNS, and are consistent with the common observation at macro-scale that an open spiral structure often has much smaller torsion rigidity and less resistance to twist buckling than a closed tubular structure. Interestingly, upon further loading after buckling onset, the torsion rigidity of the CNS (indicated by the rising slope after the load drop) becomes comparable to that of the MWCNT. This mainly results from the highly distorted and tightened cross-section of the CNS and the MWCNT at postbuckling (insets 2 and 4 in Fig. 3(a)), while the effect of topology on torsion rigidity becomes less significant. The above distinction in the deformation behaviors under torsion is also evident in CNSs and MWCNTs of various diameters (2 to 5 layers) (Fig. 3(b)). Figure 3(c) plots θ_{cr} of a MWCNT, a CNS and a SWCNT as a function of their diameter, respectively. Though in general θ_{cr} decreases as the diameter of the MWCNT, CNS, or SWCNT increases, θ_{cr} of a CNS is much lower than that of a MWCNT of the same diameter and only slightly higher than that of a SWCNT of the same diameter.

C. Buckling under bending

Bending moment is applied to a CNS (or a MWCNT) by rotating its two end surfaces out of their plane in opposite directions while keeping the contour length of the CNS (or MWCNT) center axis a constant. Figure 4(a) plots the resultant bending moment as a function of curvature for a 4-layer MWCNT and two 4-layer CNS (with different positions of its outer open edge relative to loading direction), respectively. The bending rigidity of the 4-layer CNS is slightly smaller than that of the 4-layer MWCNT. The effect of bending direction relative to the position of the free edge of the CNS on its bending deformation behavior is negligible. At the onset of buckling, two kinks set in on the compressive side of the CNS (or the MWCNT) and there is no significant drop in the resultant bending moment. The critical curvature for buckling, κ_{cr} , is then determined by the applied curvature at the onset of kink formation in the CNS and MWCNT under bending. κ_{cr} of the 4-layer MWCNT is 0.024 nm⁻¹, and that of the 4-layer CNS is 0.026 nm^{-1} or 0.023 nm^{-1} (in two loading directions, respectively). Further simulations show similar deformation and buckling behaviors of CNSs and MWCNTs with various diameters (2 to 6 layers) (Figs. 4(b) and 4(c)). The bending rigidity of a CNS increases and its κ_{cr} decreases as its diameter increases, so does that of a MWCNT. κ_{cr} of a CNS is only slightly smaller than that of a MWCNT of the same diameter. The similar bending buckling behavior of a CNS and a MWCNT can be understood as follows. While compression buckling of a CNS (or a MWCNT) results in distortion of its whole cross-section and twist buckling deforms the whole structure, bending buckling only causes severe distortion of a fraction of the cross-section near each kink. Kinks most likely initiate in the compressive side of the outermost layer of the CNS (or the MWCNT). Further development of the kinks is constrained by neighboring inner carbon layers through vdW interactions and cannot propagate further through the whole cross-section. As a result, bending buckling of the CNS (or



FIG. 4. (a) Resultant bending moment as a function of curvature for a 4-layer MWCNT (dashed line) and two 4-layer CNSs (solid and dotted lines, corresponding to two different positions of their outer open edge relative to loading direction), respectively. Insets ① and ② show the deformed shapes of the 4-layer MWCNT at a curvature of 0.025 nm⁻¹ (right after onset of buckling) and a postbuckling curvature of $0.052 \,\mathrm{nm}^{-1}$, respectively. Insets 3 and 4 show the deformed shapes of the 4-layer CNS at a curvature of $0.027 \,\mathrm{nm}^{-1}$ (right after onset of buckling) and a postbuckling curvature of $0.052 \,\mathrm{nm^{-1}}$, respectively. Color shades represent levels of potential energy. (b) Resultant bending moment as a function of curvature for CNSs (solid lines) and MWCNTs (dashed lines) of various diameters (2 to 6 layers). (c) Critical buckling onset curvature κ_{cr} of a MWCNT, a CNS, and a SWCNT as a function of their diameter, respectively.

the MWCNT) causes only rather localized kinks. In this sense, the difference in cross-section topology between a CNS and a MWCNT has negligible effect on their bending buckling behavior.

IV. A CASE STUDY OF POTENTIAL APPLICATIONS OF THE BUCKLING INSTABILITY OF CNSs

The above understanding of the buckling instability of CNSs could be potentially leveraged to enable the design of new functions of nano-devices. As a demonstration, we report a case study of molecular mass transport enabled by torsional instability of CNSs.

Previous theoretical studies have demonstrated that CNSs have the potential for hydrogen storage.^{7,8} Enthusiasm for utilizing CNSs for hydrogen storage aside, one crucial but largely unexplored issue for the success of this potential application is an effective mechanism for molecular mass transport through CNSs. For example, it remains elusive how to shuttle the hydrogen molecules adsorbed inside CNSs. To address this unexplored issue, here we demonstrate an effective mechanism of torsional-instability-enabled transport of hydrogen molecules through a CNS, inspired by recent studies of atomic transportation via carbon nanotubes.²⁷

In the simulation, a CNS of a length of 8 nm and an inner core diameter of 2 nm is initially immersed in a hydrogen reservoir whose pressure is kept at 1 MPa. The C-C covalent interaction and vdW force within the CNS are described by the same potentials defined in Sec. II. To simulate the hydrogen physisorption on the CNS, the hydrogencarbon vdW interaction is described by a Lennard-Jones atomic pair potential $V_{CH}(r) = 4\varepsilon_{CH} \left(\frac{\sigma_{CH}^{12}}{r^{12}} - \frac{\sigma_{CH}^{6}}{r^{6}}\right)$, where r is the hydrogen-carbon atomic pair distance, $\varepsilon_{CH} = 2.998$ $\times 10^{-3}$ eV, and $\sigma_{CH} = 3.18$ nm.²⁸ The simulation is carried out in LAMMPS with a time step of 0.001 ps and temperature kept at 70K. Driven by concentration gradient, hydrogen molecules are shown to enter the CNS and be adsorbed inside the CNS due to the vdW adhesion. After about 300 ps, the hydrogen physisorption process reaches equilibrium, with 572 hydrogen molecules adsorbed and adhered inside the CNS, corresponding to a gravimetric hydrogen uptake of 1.56 wt. %. Note that chemisorption of hydrogen molecules on the CNS could also occur,²⁹ which can potentially lead to a higher hydrogen storage capacity. Such an aspect is beyond of the scope of this paper and will be reported elsewhere.

To achieve the transport of these adsorbed hydrogen molecules through the CNS, a torsional deformation up to 0.17 nm^{-1} is gradually applied to the CNS by fixing the left end of the CNS and twisting its right end with a loading rate of 5.45 \times 10⁻⁴ nm⁻¹ ps⁻¹. Initial torsional deformation causes the tightening of the CNS, resulting in a decrease of the size of the CNS inner core. Decreasing space inside the CNS imposes increasing repulsive net forces on the adsorbed hydrogen molecules due to the nature of hydrogen-carbon vdW interaction. As a result, some adsorbed hydrogen molecules are pushed out of the inner core of the CNS. Figure 5(b) plots the evolution of the amount of the adsorbed hydrogen molecules inside the CNS as a function of the applied torsional deformation. At the onset of the torsional buckling at 0.031 nm^{-1} (Fig. 5(c)), about 14.5% of the adsorbed hydrogen molecules have been pushed outside of the CNS. The torsional buckling causes the CNS to collapse, leading to a significant decrease of the size of the CNS inner core (e.g., Fig. 5(d)). Consequently, as the torsional buckling develops, much more adsorbed hydrogen molecules are squeezed out of the CNS, as indicted by the steeper slope of the curve in Fig. 5(b) after onset of buckling. For example, at a twisting angle of 0.105 nm^{-1} (Fig. 5(d)), more than 60% of the adsorbed hydrogen molecules are pushed out of the CNS. At the end of the twisting deformation of 0.17 nm^{-1} , 79.4% of the hydrogen molecules initially adsorbed inside the CNS can be squeezed out of the CNS, suggesting the high efficacy of a molecular mass transport mechanism via a CNS enabled by its torsional buckling instability. Previous studies show that alkali doping can increase the interlayer distance of a CNS, leading to further enhancement of the capacity of CNS-based hydrogen storage.⁷ An alkali doped CNS also buckles when subject to severe twisting deformation, therefore the hydrogen transport mechanism enabled by the CNS torsional buckling instability demonstrated above still holds,



FIG. 5. (a) Resultant torque as a function of twisting angle per unit length for an 8 nm long CNS with hydrogen molecules adsorbed inside. (b) Percentage of hydrogen molecules remaining inside the CNS as a function of twisting angle per unit length. After the occurrence of torsional buckling, the collapse of the CNS squeezes more adsorbed hydrogen molecules out of the CNS, as indicated by the change of slope of the curve in (b). (c) and (d) show the side and end views of the CNS (green) and the hydrogen molecules (red) initially adsorbed inside the CNS inner core at the onset of torsional buckling and at a twisting angle of $0.105 \, \text{nm}^{-1}$, respectively. For visual clarity, the hydrogen molecules initially outside of the CNS are not shown.

given the similar nature of the vdW interaction between the adsorbed hydrogen molecules and the doped CNS.

V. SUMMARY

Systematic molecular mechanics simulations are carried out to study the buckling instability of CNSs under axial compression, torsion, and bending. The unique open topology of CNSs and the existence of two free edges in CNSs produce distinct features of buckling instability from those of MWCNTs. These results could provide a better understanding of the mechanical reliability of CNS-based electromechanical devices. The distinct buckling features of CNSs could shed light on designing new functions of nanoscale devices. As a case study, we demonstrate an effective mechanism of molecular mass transport via a CNS enabled by its torsional buckling instability, which can potentially facilitate the future application of CNS-based hydrogen storage. Furthermore, the highly durable and elastically deformable basal graphene suggests reversible buckling of the CNS under cyclic loading (as supported by the fact that, in all our simulations, no C-C bond breaking is observed under various types of post-buckling deformation), another desirable feature for CNS-based device applications. We therefore call for further theoretical and experimental demonstration of potential applications enabled by the buckling instability of CNSs.

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