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\textbf{ABSTRACT}

The insights into transport behavior and the effects of bending on heterostructures constructed from boron nitride (BN) and carbon (C) nanotubes are important for their flexible device applications because the two systems have equally excellent mechanical but completely different electrical properties. In this work, coaxial BN–C nanotubes have been fabricated and their intrinsic transport properties, as well as structural and electrical response to bending deformation, are studied inside a high-resolution transmission electron microscope. Ballistic, diffusive, and hopping transports within different tube length ranges have been observed. When bending deformation was applied to the tubes, although severe kinking becomes apparent, their transport properties are not notably affected. Meanwhile, both theoretical and experimental analyses confirm that the kink positions depend on the ratio of tube diameter to its length. Possible formation of quantum dots, directly within the kink areas, was predicted through calculations of electron density redistribution between nanotube walls at bending.

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I. INTRODUCTION

Over the last several years, flexible devices have attracted tremendous attention due to various potential applications in electronic devices, sensor chips, and photodetectors. Thus, the mechanical elasticity, structural changes, and electrical transport of the constituting materials under cycling bending are of crucial importance with respect to reliable practical applications. Boron nitride nanotubes (BNNTs) and carbon nanotubes (CNTs) have intensively been studied and are currently regarded as materials of choice for many structural applications; they reveal extremely high Young’s modulus, high fracture strength, and excellent flexibility. By contrast, they have just the opposite electrical characteristics, i.e., BNNTs are insulators, whereas CNTs are metals or semiconductors depending on the tubes’ helicity. It is worth noting that BNNT electrical properties are rather difficult to tune. This fact results in blocking their possible applications in flexible stress sensors or switches. Thus, it is of great interest and challenge to modify BNNT electrical response and create nanostructures having a tunable percolation threshold and to facilitate their applications in flexible electronics. Actually to date, both theoretically and experimentally, tremendous efforts have already been put to modulate the transport behaviors of BNNTs, using doping, strain engineering, heterostructure design, structure unwrapping, etc. Another prospective approach is to fabricate BN–C heterostructures, usually regarded as nanoscale “Lego” blocks, and provide the engineers with diverse possibilities for tuning properties and promoting advanced applications. For instance, Xiang et al. have reported on a design of BN/C van der Waals heterostructures, showing the similar transport behavior to bare CNTs, but much better thermal stabilities of the material. Jing et al. developed the C@BN nanotube arrays and revealed the enhanced shape recovery and improved compressive strength. These reports clearly demonstrate the interesting potentials of BN–C related composites. However, many questions still remain not answered, e.g., (i) What kind of transport properties such heterostructure would have? (ii) What are the bending effects on their electrical behavior? (iii) How such heterostructures would bare a heavy bending deformation? (iv) Would BN and C tubular domains separate or their interface break under bending; and if yes, how this would affect the overall structural integrity and physical properties? All these issues call for a direct study of bending deformation of coaxial hybrid BN–C nanotubes.

Herein, we have designed and synthesized core-shell coaxial BN–C nanotubes and applied an in situ transmission electron microscopy (TEM) technique to study their transport characteristics and the effects of external bending deformation on their structural evolution and electrical transport. Ballistic transport within the tube contact lengths of ~250 nm, diffusive transport within the lengths ranging from 250 nm to 750 nm, and the hopping transport for the larger lengths have been documented. When a bending deformation has been applied, all these three transport modes are not notably affected, while a peculiar kinking deformation is observed. It has been found that the kink positions are strictly related to the structural nanotube parameter, i.e., a ratio between the tube diameter and its length. Interestingly, after deformation, BN–C nanotubes have fully recovered, even after very high angles of bending, without any traces of failure or structural defects appearance, showing excellent electrical and structural stability. Combination of in situ TEM and molecular dynamic (MD) simulations has then provided us with an effective way to uncover the transport and mechanical behaviors of composite BN–C nanotubes and paved the way toward their realistic and smart applications in flexible electronics.

II. RESULTS AND DISCUSSION

Coaxial BN–C hybrid nanotubes were synthesized via a threestep high-temperature process. First, pure BNNTs were prepared by the boron and metal oxide-assisted chemical vapor deposition (BOCVD) method in an induction furnace, followed by a high temperature purification process at 1800 °C. Subsequently, carbon coating was deposited on tubes via a CVD method by using hexane as a carbon source and Ar as a carrier gas. This process was conducted in a horizontal electrical furnace under ambient pressure, at 1100 °C for 60 s. Finally, the carbon-coated BNNT samples were annealed at 1800 °C for 6 h to induce complete graphitization and to remove possible impurities. A typical TEM image, shown in Fig. 1(a), reveals a hollow one-dimensional structure which perfectly maintains its structural integrity even after the employed high-temperature synthesis. The corresponding high-resolution TEM (HRTEM) image of the tube walls is depicted in Fig. 1(b). The distance between the adjacent tubular layers is ~0.33 nm over the whole structure, implying its excellent crystallinity. Electron energy loss spectroscopy (EELS) maps were created to confirm the overall composition and spatial distribution of the constituting elements. Figure 1(c) depicts an annular dark field (ADF) scanning TEM (STEM) image of segment from a different nanotube, and Figs. 1(d)–1(f) present the corresponding elemental spatially resolved EELS maps for constituting elements. EELS mapping unambiguously confirms the coexistence of B, N, and C species within the nanotube walls. It is worth noting that the C signal becomes more intense on the tube periphery, suggesting that C layers form the outer shells. This is further confirmed by the EEL spectra extracted from the different regions in Fig. 1(c), as shown in Fig. 1(g). In regions “1” and “3,” only peak at 284 eV originated from C is recognized, while in the middle area “2,” three distinct peaks are seen at 188 eV, 284 eV, and 401 eV, corresponding to the K-shell ionization edges of B, C, and N, respectively. The peaks reveal sharp π* features and σ* bands and imply typical sp2 bonding configuration. The atomic ratio from the EELS data (region “2”) is calculated as B:C:N = 1.00:0.36:0.94. Elemental composition for the core and shell was further verified by comparative EEL spectra analysis on the same nanotube before and after the annealing process. The results showed that only the peaks for B and N remained after thermal treatment, indicating that the core is made of the pure BN (see more details in the supplementary material; Fig. S1). All these results confirm that as-obtained samples are sandwichlike coaxial BN–C tubular nanostructures.

Transport behavior of nanotubes with uniform C coating as a function of tube length was first studied. The schematic of the experimental setup and TEM image showing the measurement process are presented in Figs. 2(a) and 2(b), respectively. Representative I–V curves at different contact lengths were recorded by moving the W probe to contact the different segments of the selected BN–C nanotube, as illustrated in Fig. 2(c). Clearly, all these I–V curves reveal a linear characteristic. However, the current values vary a lot at different contact lengths. Then, we evaluated the resistance of a nanotube (Rn) as a function of the contact length. For the
present two-terminal contact measurements, the total resistance $R$ is the sum of three contributions: $R_g$, $R_w$, and $R_n$, where $R_g$ and $R_w$ are the contact resistances of a nanotube to the gold wire and W probe, respectively. $R_g$ may vary from one BN–C nanotube to another, but it is constant for a selected nanotube, whereas $R_w$ may fluctuate between two individual contact experiments, albeit such fluctuation is rather small. Figure 2(d) presents the evolution of the nanotube resistance along with contact length change as acquired from $-100$ mV to $+100$ mV, the value excludes the contact resistances $R_g$ and $R_w$, ranging from 9.5 kΩ to 17.5 kΩ, as evaluated from different BN–C nanotubes (see more details in the supplementary material; Fig. S2). The plot shows that $R_n$ increases sharply from 11.3 kΩ at 90.3 nm to 1110.3 kΩ at 809.8 nm and displays a nonlinear behavior. Interestingly, combining the enlarged region with contact length smaller than 476.9 nm and considering the whole plot, one may conclude that the relationship between the tube resistance and the contact length can be divided into three definite areas, i.e., (1) resistance values lower than 12.9 kΩ within the contact lengths smaller than 233.7 nm, which can be considered as the ballistic transport (region 1); (2) resistances increasing linearly with the contact lengths, from 292.7 nm to 476.9 nm, corresponding to a diffusive transport (region 2); and (3) resistances increasing exponentially (see the exponential fitting) under further length increasing, up to $\sim$930.4 nm, which can be ascribed to a hopping mechanism. These regions correspond to three different transport regimes. In the case of ballistic transport, carriers easily travel within the length range
corresponding to the mean free path \( l \). Within this contact length range, the resistances are independent of the contact length. For a single channel medium, the resistance of the ballistic conductor is given as \( R = \frac{h}{2q} \approx 12.9 \text{ k}\Omega \) (where, \( h \) is Planck’s constant and \( q \) is the electron charge). At scales longer than \( l \), the electrons will be elastically scattered and the transport becomes diffusive. Within this range, the resistance is linearly dependent on the contact length and can be approximately expressed as \( R \approx \rho \frac{L}{S} \) (where, \( \rho \) is the resistivity, \( L \) is the contact length, and \( S \) is the cross-sectional area).\(^{24}\) Our previous work has verified that with longer distances, instead of a uniform coating made of carbon shells, the tubes are covered by small carbon islands. Thus, under further increasing of the contact length, electron hopping from one island to another becomes dominant and the resistance shows an exponential dependence on the length.\(^{26}\) The observed nonlinear dependence of \( R_n \) indicates that the electronic transport over the whole tube is not Ohmic and the electron-defect interactions are the main source of resistance, i.e., the electrons suffer from the scattering events with defects inside the conductor.\(^{30}\) Our previous work has verified that \( R_n \) indicates that the electronic transport over the whole tube is not Ohmic and the electron-defect interactions are the main source of resistance, i.e., the electrons suffer from the scattering events with defects inside the conductor.\(^{30}\)

\( I-V \) measurements on different BN–C nanotubes also show the similar resistance vs contact length plots although the ballistic and diffusive transport ranges differ for different BN–C nanotubes (see more details in the supplementary material; Fig. S3). This fact can be ascribed to different patterns of defect distributions in each particular nanotube. The above experiments imply that the nonlinear resistance vs contact length is a common intrinsic phenomenon for the present coaxial BN–C nanotubes.

The experiments clearly show that the transport in BN–C nanotubes is remarkably enhanced as compared to pure BNNTs, which are electrically insulating. For the potential applications in flexible electronics a stable transport is undoubtedly preferable. To understand how the external mechanical deformations influence the atomic structure and electrical properties, the structural evolution observations in-tandem with in parallel \( I-V \) curve recording and tube resistance measurements were performed under \textit{in situ} bending in TEM (Fig. 3). A series of TEM images, shown in Fig. 3(a), illustrates a structural evolution during deformation. Under moving the W probe forward, the hybrid BN–C nanotube first undergoes structural changes via generation of a sharp kink, instead of an uniform arclike tube bending as a whole.\(^{27}\) Once the kink appears, further deformation develops via increasing the kink angle, which can reach a value of up to \( \approx 67.2\degree \). The corresponding \( I-V \) curves recorded at different bending angles are presented in Fig. 3(c), showing that the output current only marginally changes (from \( \approx 1.1\% \) to \( 7.2\% \)). Such small variations can be ascribed to the slight contact condition changes (between the W probe and the nanotube). Importantly, although both core BN and covering C layers are severely deformed and intertwined [Fig. 3(b)], the kink immediately disappeared and the nanotube entirely recovered to its initial state (both structurally and electrically) once the probe had been retracted (see more details in the supplementary material; Fig. S4). Thus, neglecting the marginal contact changes, the present BN–C tube shows quite stable transport behavior under bending. Figure 3(d) depicts the relationship between resistances and bending angles of the nanotubes showing different transport characteristics. No matter what type of transport is dominating, i.e., the ballistic, diffusive, or hopping, the resistances vary within a very small range, implying that the deformation does not dramatically enhance carrier scattering (see more details in the supplementary material; Fig. S5). In addition, comparative studies on the transport properties of BNNTs and CNTs as a function of the contact length, as well as the bending angles, were conducted. The results showed that the insulating characteristics of BNNTs are independent on the contact length or bending angles. In terms of CNTs, only ballistic and diffusive transport modes were obtained at different contact length regions and their transport behaviors were also not severely affected by bending deformation (see more details in the supplementary material; Fig. S6).
Fig. S6). These results indicate that the present BN–C heterostructures should be of advantageous use for novel flexible devices which can withstand exceptionally high bending strains.

To obtain fundamental insights into both electrical and mechanical properties of hybrid BN–C nanotubes under external loading, direct simulation of the bending process was performed. Unlike CNTs, BNNTs may have a polygonal cross section caused by interlayer electrostatic interactions that are sufficient to induce the interwall correlation, which will undoubtedly affect their mechanical and electronic properties. Thus, first, we studied in detail the features of the atomic structure of hybrid nanotubes having a BNNT core and a CNT shell (Fig. 4). Here, we considered only “zigzag” nanotubes; due to the fact that in the previous studies, it was predicted that only zigzag nanotubes could form a polygonal cross section, while, in case of the armchair and chiral nanotubes, polygonization could change and even disappear. Theoretical calculations show that the polygonal shape of the BN core is transmitted to the outer C layers. As a result, external CNT cross section also becomes a polygon.

Our calculations show that the polygonal shape of the inner BNNT influences the C shell only up to four outer C layers. After 4 layers, the outer shell polygonization effect mostly vanishes.

In addition to changes in the atomic structure, the polygonization effect can affect the mechanical properties of hybrid nanotubes. The presence of edges in the structure of polygonal nanotubes can initiate anisotropy in behavior under mechanical loading. Therefore, we performed MD calculations of transverse compression of hybrid BN–C nanotubes in various directions and found that the formed polygons only slightly influence the hybrid tube behavior under external transverse mechanical stresses (the slopes of the curves are similar; see more details in the supplementary material; Fig. S7).

We then elucidated the behavior of hybrid coaxial BN–C nanotubes under bending at the atomic level by performing large-scale MD simulations. We studied hybrid structures with various diameters, lengths, and the number of layers. Close to the experimental procedure, we considered the stepwise tip movement, which is associated with the consecutive movement of the tip in the horizontal direction and, then, in the vertical direction. In order to directly compare our calculation results with the experimental data on the same plot, we used a dimensionless $D/L$ ratio between tube diameter ($D$) and its length ($L$). According to experimental data in the considered model, one end of the tube was fixed, while the force was applied to another end. In this case, the length of the tube and the applied force position are both defined as $L$. It should be noted that during test calculations, it was found that the shift of the tip position leads to the variation of the kink position. The shift of the applied force toward the fixed end of the tube allows us to consider such process similarly to a bending process of the shorter hybrid tube. Such parameter allows us to analyze properties of structures with sufficiently different sizes and, therefore, is very useful in the comparison between larger experimental structures and studied computational models. Figures 5(a) and 5(b) show two hybrid

![FIG. 4. Atomic structure of a hybrid BN–C nanotube (cross-sectional view, BN-blue, C-green) before (a) and after (b) geometry relaxation.](Image)

![FIG. 5. Main steps of a hybrid BN–C bending process exemplified by coaxial nanotubes with 2 inner BN layers and 2 outer C layers (diameter of 2.8 nm) with a length of (a) 17 nm and (b) 45 nm. Schematic representation of the external acting force is presented by red arrows; (c) Experimental TEM images of bent hybrid BN–C nanotubes with various lengths and diameters. (d) Dependence of the $L_{kink}/D$ ratio on the $D/L$ ratio for hybrid nanotubes. Calculated and experimental data are shown by red and blue symbols.](Image)
nanotubes with the same number of C and BN layers (2 C layers and 2 BN layers) but with a difference in the D/L ratio (0.16 and 0.08). Under the stress loading process, in case of a smaller D/L value, a nanotube kink ($L_{\text{kink}}$) appears closer to the nanotube center, while the kink for the tube with a larger D/L value is located closer to the fixed end. General correspondence of theory with the experiments is illustrated by the recorded BN–C nanotubes bending processes in Fig. 5(c). Even at the critical ratio of bending, there are no defects formed [Figs. 5(a) and 5(b)]. This simulation results suggest the reason behind the excellent structural flexibility during bending. In Fig. 5(d), the dependence of the nanotube kink position, described as the $L_{\text{kink}}/D$ ratio on the D/L ratio, is presented. Here, the calculated data obtained from MD calculations (red circles) show the behavior of small hybrid nanotubes, whereas experimental data expand this dependence toward the larger nanotubes (blue squares). Red dots correspond to theoretical results of the kink position estimation for hybrid nanotubes with a various number of layers varied from 4 to 9 (from 2 BN and 2 C to 3 BN and 6 C layers). With decreasing D/L ratio, the kink position monotonically shifts and approaches the middle of the tube. Based on MD simulations, it could be concluded that the main geometrical parameter, which is responsible for the kink position during bending, is indeed the D/L ratio. This fact originates from a competition of the moment of inertia and nanotube bending stiffness. Moreover, decreasing the number of inner BN layers within hybrid BN–C nanotubes does not lead to the changes in the position of the kink, while the overall mechanical response could be significantly different.

Significant bending of hybrid BN–C nanotubes can significantly impact their local electronic properties in the vicinity of a kink region (Fig. 6). We found that in the critical bending regime, the distance between the layers in the multilayered hybrid nanotubes significantly decreases (from 3.35 Å to 2.17 Å), but the misorientation of atomic layers hinders the phase transition activation. The reduction tendency of the interlayer distance in the kinking regions was further confirmed by the HRTEM observations (see more details in the supplementary material; Fig. S8). Nevertheless, such a phenomenon leads to strong redistribution of electronic density between layers, which contribute to the formation of local conductive channels near the kink area [Fig. 6(a)]. Indeed, systematic study of electron density evolution upon decreasing the regarded distance for the case of 2 C layers covered on 2 BN layers shows strong charge redistribution and joint electron density between the layers when the distance is reduced to 2.17 Å. In Fig. 6(b), the electron density distribution in the e/Å$^3$ units between C and BN layers upon the interlayer distance decrease is presented. In Fig. 6(a), we show a slice of electron density in the middle of a coaxial BN–C tube. Formation of the joint electron density from all layers of BN–C tubes from the inner side of the kink area is apparent. Strong interaction between the layers is also observed within the kink area, thus shrinking the distance. Such a reduction in the distance between the nanotube walls could lead to an interesting physical property change via the formation of quantum dots in the kink regions. Such phenomenon may be important for future applications of the present hybrid nanotubes in advanced optical and optoelectronic fields.

III. CONCLUSION

In summary, we designed core-shell hybrid BN–C nanotubes and studied their mechanical and electrical properties under bending to further promote their potential applications in flexible devices. In situ TEM investigations revealed that such nanotubes possess a nonlinear transport behavior along their lengths. The effects of peculiar kinking deformation on both structural and electrical parameters were analyzed in detail. It has been found that even when the sharp kinks appeared, the transport behavior was not notably affected. Importantly, the tubes could fully recover their shape after bending, implying their excellent structural flexibility. Computations showed that the kink positions had closely been related to the tube geometrical parameter, i.e., tube diameter to its length ratio, which is in good agreement with the in situ TEM bending tests. In the meantime, analysis of atomic structures in the kink area confirmed the absence of permanent structural defects and full structural recovery of the tubes. Bending led to significant redistribution of electron density between the layers which could be directly connected with the formation of quantum dots in the kink regions.

IV. METHOD

A. Materials synthesis and characterization

Tubular BN–C heterostructures were synthesized via a three-step chemical vapor deposition (CVD) method, which is described in our previous work in detail. 1–4 TEM imaging and electron energy
loss spectra (EELS) mapping of individual BN–C nanotubes were performed using a JEOL 3000F TEM, by using an in situ heating holder to alleviate/avoid the possible contamination during the scanning process.

B. In situ TEM experiments

In situ bending experiments on individual coaxial BN–C nanotubes were performed inside a JEOL 3100FF (Omega filter) TEM by using a scanning tunneling microscopy-TEM holder (Nanofactory Instruments AB). Hybrid BN–C nanotubes were firmly attached to the edge of a flat Au wire using conductive silver epoxy, and a freshly electrochemically etched W probe was used as the counter electrode. The W probe was controlled by a piezomotor to contact the selected nanotube and to record the current-voltage (I–V) curves. Bending deformation of the BN–C nanotubes was initiated by moving the W probe forward (after the two sides of the setup had physically contacted each other); thus, the bending angles could be traced and precisely measured at every stage of deformation.

C. Computational details

To describe the features of a possibly polygonal cross section of hybrid coaxial BN–C nanotubes and to further study the atomic structure of CNT layers wrapped around a BNNT core, a newly developed potential of interlayer interaction based on ReaxFF was used.\(^1\)\(^2\)\(^3\) This potential contains three terms describing the interlayer attraction due to dispersive interactions, repulsion due to anisotropic overlaps of electron clouds, and, also, monopolar electrostatic interactions. Simulations of the bending process were carried out by means of molecular dynamics calculations based on the program software LAMMPS.\(^3\) We simulated hybrid BN–C nanotubes with various diameters, lengths, and the ratios between the number of C and BN layers. Bending of hybrid coaxial nanotubes was modeled via interaction with an atomic force microscopy tip which pushed the structure with a step of ~1.4 Å. Interactions between the tube and the simulated tip were described with a purely repulsive force. Before the mechanical test and at each bending step, the system was annealed at a temperature decreasing from 300 to 10 K, while the maximum interatomic forces became less or equal to 0.05 eV Å\(^{-1}\). Annealing time at each step was chosen as 3.5 ps with the time step of 10\(^{-3}\) fs. The atomic structure of considered hybrid nanotubes contained 5 × 10\(^4\) to 6 × 10\(^5\) atoms in total. The atomic interactions between B and N atoms in a BNNT were described by the Tersoff 3-body potential implemented in LAMMPS.\(^3\) We simulated hybrid BN–C nanotubes with various transport behaviors at different bending deformation.

SUPPLEMENTARY MATERIAL

See the supplementary material for the contact resistance evaluated from different BN–C nanotubes, resistance vs contact length plots for different nanotubes, I–V curve and TEM image revealing that the BN–C nanotube fully recovers both structurally and electrically after severe deformation, variation of AR for different BN–C nanotubes with different transport behaviors at different bending angles, geometries of hybrid BN–C nanotubes before and after transverse compression with different load directions, and the dependence of the strain energy of nanotube on the strain.

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