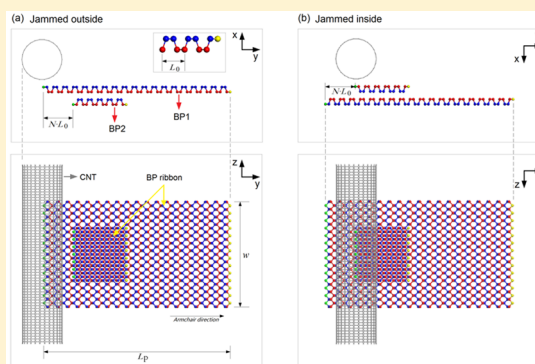


Self-Assembly of a Jammed Black Phosphorus Nanoribbon on a Fixed Carbon Nanotube

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ABSTRACT: Nanotube synthesizing from black phosphorus (BP) is still challenging in laboratory. Fabricating a BP nanotube by self-assembling of a BP nanoribbon seems promising. To estimate the feasibility of such fabrication method, this study performs numerical experiments of self-assembling a jammed BP ribbon on a fixed carbon nanotube using molecular dynamics simulation. The study is based on the following two facts: The phosphorus–phosphorus (P–P) bond is weaker than the bond of carbon–carbon (C–C) and the van der Waals interaction among nonbonding phosphorus atoms is stronger than that between phosphorus atoms and carbon atoms. The results show that when a longer BP ribbon is jammed by a shorter BP ribbon the self-assembling result depends on the relative positions of carbon nanotube (CNT) and the two BP ribbons. Only when the shorter BP ribbon is on the outside of the longer ribbon can the longer BP ribbon be wound on the CNT to form an ideal BP nanotube. The finding is helpful for practical applications of BP nanotubes in nanodevices.



1. INTRODUCTION

Few-layered black phosphorus (BP), as a typical 2D material, has attracted much attention due to its excellent physical properties in recent years.^{1–6} Up to now, few-layered black phosphorene has been fabricated and shaped into some nanodevices experimentally.^{7–9} Inspired by the construction of carbon nanotube (CNT)^{10–14} and graphene,^{15–18} researchers may naturally think that a nanotube from a single-layered black phosphorene could exist.^{19,20} So far, such a BP nanotube has not been discovered even in laboratory. It is mainly due to the following two facts. One is the phosphorus–phosphorus (P–P) bonds in BP are much weaker than those in graphene.²¹ These weaker bonds are more sensitive to its ambient temperature and pressure. Mutual transformation among phosphorus allotropes is the evidence supporting this fact.^{22,23} Another is that each layer of BP has two surfaces with a distance of only ~ 0.2 nm, leading to the area inertia of moment with respect to out-of-plane bending stiffness of a single-layered BP (SLBP) much larger than that of a single-layered graphene. If, for example, synthesizing a phosphorus nanotube just from phosphorus atoms by self-assembling,^{24–27} then the bond length in the outer surface of BP nanotube would obviously be higher than that in the inner surface. Consequently the potential energy of an atom either in the outer surface or in the inner surface of BP nanotube would obviously be greater than that of an atom in BP.^{28,29} This situation hardly appears in a process of self-assembling.

The nanotube of BP has two significant merits considering their structural stability and electric property. One is that the

unsaturated phosphorus atoms on the tube are confined at both ends of the tube, which is significant for avoiding chemical reaction with water or oxygen molecules.^{30,31} Another is that the BP nanotube behaves as an excellent semiconductor with a wider range of band gaps than CNT.²⁰ For an NEMS (nanoelectromechanical system) requiring a 1D component with good semiconducting property, BP nanotube would be an ideal candidate material.

The challenge for obtaining a phosphorus nanotube by directly self-assembling phosphorus atoms motivates us to explore other methods. Four reasons motivate us to try a new approach for fabricating a BP nanotube by winding a SLBP on a CNT. The first is that a SLBP nanoribbon can be easily obtained in laboratory. The second is that a SLBP is able to curve at a large rotational angle along its armchair direction.^{28,29} The third is that the interaction among nonbonding phosphorus atoms is much stronger than that between phosphorus and carbon atoms,³² which means that the new BP nanotube on CNT can be removed from the CNT without damage.³³ Besides, the BP nanotube can move into a CNT with a larger radius for the protection from water or air.^{30,31,34,35} Last, the self-assembly approach has been widely studied and used in the field of nanotechnology. With the approach, we can demonstrate that a pure SLBP may be difficult to obtain because it could attract some adjacent fragments in fabrication.

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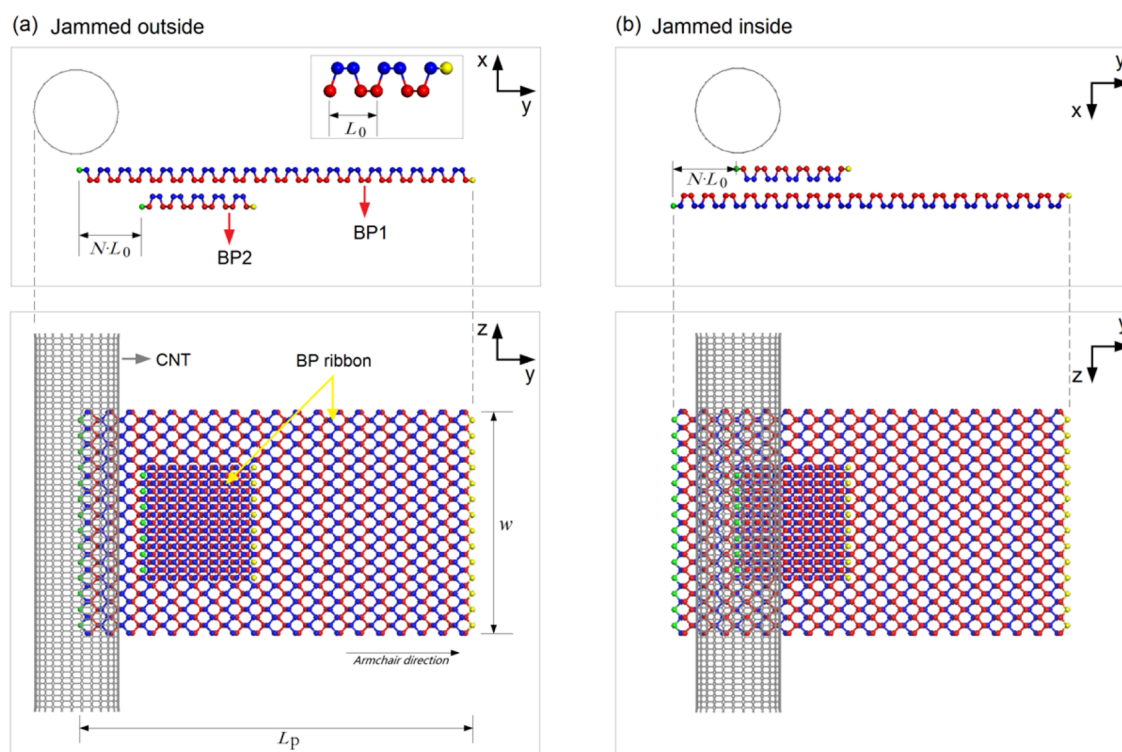


Figure 1. Schematic of a longer black phosphorus ribbon (BP1) jammed with a shorter BP ribbon (BP2) near a fixed CNT (13, 13) with hydrogenated ends. (a) BP2 is outside BP1. (b) BP2 is inside BP1. Tube axis is directed along the positive z axis. Armchair direction of BP ribbon is initially along the y axis. L_0 (≈ 0.44 nm) is the unit length of BP ribbon along the armchair direction. L_p ($\approx 19L_0 \approx 8.24$ nm) is the perfect length of BP1, and the width of BP1 is w (≈ 4.64 nm). The length and width of BP2 are ~ 2.34 and ~ 2.32 nm, respectively. The initial distance along the armchair direction between the left ends of BP1 and BP2 is N times L_0 . $N = 0, 1, 2, 3, 4$, and 8 are considered in the discussion. The normal distance between BP1 and BP2 is ~ 0.344 nm. The distance between CNT and BP1 in panel a or BP2 in panel b is the equilibrium distance, that is, 0.342 nm. For convenience, the edge atoms are in green (left side) or yellow (right side).

Hence, in this study, we will investigate the self-assembling of a longer BP ribbon jammed with a shorter BP ribbon on a fixed CNT. In the simulations, the shorter BP ribbon behaves as a fragment in fabrication.

2. MODELS AND METHODOLOGY

In Figure 1, a longer BP ribbon (BP1) is initially jammed by a shorter BP ribbon (BP2) when BP1 is put near a CNT for nanotube generation. BP2 is outside BP1 in Figure 1a or inside BP1 in Figure 1b. L_p , the length of BP1, is the perfect length with which BP1 can be wound and finally form a perfect nanotube on the CNT. To investigate the influence of BP2 on the winding process of BP1, the edge distance along the z axis between the two sides of BP1 and BP2 is equal. The y directional distance between the left edges of BP1 and BP2 is N times L_0 . N varies from 0 to 9. At each end of CNT, there are four rings of carbon atoms fixed with their degrees of freedom in simulation.

The geometric parameters involved in the present study are chosen based on the following considerations: (1) The size of fragment (BP2) is estimated on the nanofabrication precision, which is ~ 1 nm. (2) The width of BP1 (to be wound and formed into a nanotube) is determined by both the width of BP2 and the cutoff of L-J potential (~ 1.0 nm). It should satisfy that the initial interaction between the adjacent edges of both BP ribbons is negligible. (3) The length of CNT depends on both the width of BP1 and the cutoff. (4) The length of BP1 depends on the radius of CNT and the balance distance

between CNT and BP (~ 0.34 nm), that is, $L_p = \sim 2\pi(r_{\text{CNT}} + 0.3422)$ nm.

Noting that the two ribbons are very close to the fixed CNT, for example, the distance between them is less than the cutoff of the L-J potential function, they are attracted by the CNT. Because of the strong attraction between BP ribbons and the CNT, BP ribbons may be curved and wound on the surface of CNT. However, the ribbons are stiff to against curvature. Besides, the attraction of CNT on ribbons is sensitive to their distance. If the longer ribbon, that is, BP1, is jammed by the shorter ribbon, then it could hardly be curved and further attached to CNT. To investigate the final stable configuration of the ribbons, the molecular dynamics simulation approach with open source code LAMMPS^{37,38} is employed. In the simulation, the bonding interaction between carbon or hydrogen atoms in the CNT is determined by the AIREBO potential.³⁹ The strength of covalent bonds between phosphorus atoms in BP ribbons is estimated using the Stillinger–Weber potential,⁴⁰ in which the parameters for phosphorus nanostructure were recently reported in ref 41. The nonbonding interaction among the CNT and ribbons is described using the 12–6 formed L-J potential, and the related parameters are listed in Table 1. Parameters for P–C interaction presented by Jiang and Park⁴² are used in this work.

In our simulation, the time step is taken to be 0.001 ps. The system made from CNT, BP1, and BP2 is first relaxed under a canonical (NVT) ensemble. The temperature T is assumed to be 8 K. A Nosé–Hoover thermostat⁴³ is employed for controlling the temperature of system. Before BP1 is wound

Table 1. Parameters in the Lennard-Jones (L-J) Potential Function³⁶ $V(r_{ij}) = 4\epsilon[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^6]$ between any Two of C, P, and H Atoms^a

atom <i>i</i>	atom <i>j</i>	σ (nm)	ϵ (eV)
P	C	0.34225	0.006878
P	P	0.3438	0.015940
C	C	0.3400	0.002844
C	H	0.3025	0.002065
H	H	0.2650	0.001499

^a $\epsilon_{\text{P-P}}$ is the highest in all cases, which indicates the strongest van der Waals (vdW) interaction among nonbonded phosphorus atoms.

on CNT, the system needs relaxation. To avoid BP1 moving toward CNT in relaxation, we fix the (yellow) atoms at the right end of BP1. From the viewpoint of experiment, BP ribbons should be fabricated and pulled to nearby a fixed CNT. Fixing either the ends of CNT or the right end of BP1 reflects the true experiment ambient in our simulations. Without fixing the CNT, it can have translational motion or rotation, which is hard for fabricating a BP nanotube from BP ribbons. If only CNT is fixed, then the BP ribbons will be attracted to CNT before it has full relaxation. According to our results, shown in Figure 2b or Figure 7, the BP ribbons are attracted and curved upon the CNT within half of a nanosecond. The motion even lasts seconds, which is much longer than the duration of the case in which the right end of BP1 is fixed. After 500 ps of relaxation, we release BP1 and start 5000 ps of running at the NVT ensemble. During running, the potential energy of the system, kinetic energy of each component, and positions of atoms is recorded for postprocessing.

For a self-assembling system, the potential energy of the system determines its state and configuration. Hence, the variation of potential energy (VPE) of a system is useful for estimating the variation of its configuration. In the present system, the potential energy of a system contains three major parts. The first is the potential energy of each component, that is, P_{C} of CNT, P_1 of BP1, and P_2 of BP2. The second is the potential energy of two adjacent components, that is, $P_{\text{C-1}}$ between CNT and BP1, $P_{\text{C-2}}$ between CNT and BP2, and P_{1-2} between both BP ribbons. The final part is the potential energy

among components, that is, $P_{\text{C-1-2}}$. So the total potential energy of the system yields

$$P_{\text{total}} = P_{\text{C}} + P_1 + P_2 + P_{\text{C-1}} + P_{\text{C-2}} + P_{1-2} + P_{\text{C-1-2}} \quad (1)$$

In the simulation, the interaction among the three components (CNT, BP1, BP2) obviously influences the six items in eq 1. For example, because of the attraction between CNT and BP ribbons, CNT may vibrate, which leads to the deformation of the tube. Then, the value of P_{C} varies simultaneously. The two ribbons are attracted by CNT and have deformation, which leads to the variation of P_1 and P_2 . The interaction between the two deformed ribbons results in the variation of P_{1-2} . When N is small, that is, the left ends of both ribbons are very close, the relative motion between the two ribbons also leads to variation of P_{1-2} , while $P_{\text{C-1-2}}$ is sensitive to the jammed type or the relative position of BP1 and BP2 and CNT. For example, when BP1 is outside-jammed by BP2 (see Figure 1a), the distance between each phosphorus atom on BP2 and CNT is ~ 0.9 nm, which is slightly lower than 1.0 nm. Hence the interaction between BP2 and CNT is very weak and the value of $P_{\text{C-1-2}}$ is very small as well. As a result, the variation of $P_{\text{C-1-2}}$ is very small as well. If BP1 is inside-jammed by BP2, then more phosphorus atoms on BP1 than those on BP2 will be kept away from the CNT at a distance no less than 0.9 nm. Hence, the value of $P_{\text{C-1-2}}$ is very small. However, if the relative motion between the two ribbons occurs, then the variation of $P_{\text{C-1-2}}$ could be higher than that in the outside-jammed model. A detailed discussion of the VPE together with the related numerical results is given in the next section.

An important situation should be mentioned here because the number N has great influence on the VPE of system. In the models shown in Figure 1, the phosphorus atoms at the edges of both ribbons are only covalently bonded with two other phosphorus atoms. Hence, new phosphorus–phosphorus (P–P) bonds may be generated among the edge atoms. If both edge atoms bonded together are on BP1, that is, a new phosphorus nanotube is formed from the wound BP1, then the value of P_1 has an obvious change. If the new bond connects both BP ribbons, then the value of P_{1-2} varies obviously. According to the data from the works in refs 44 and 41, the

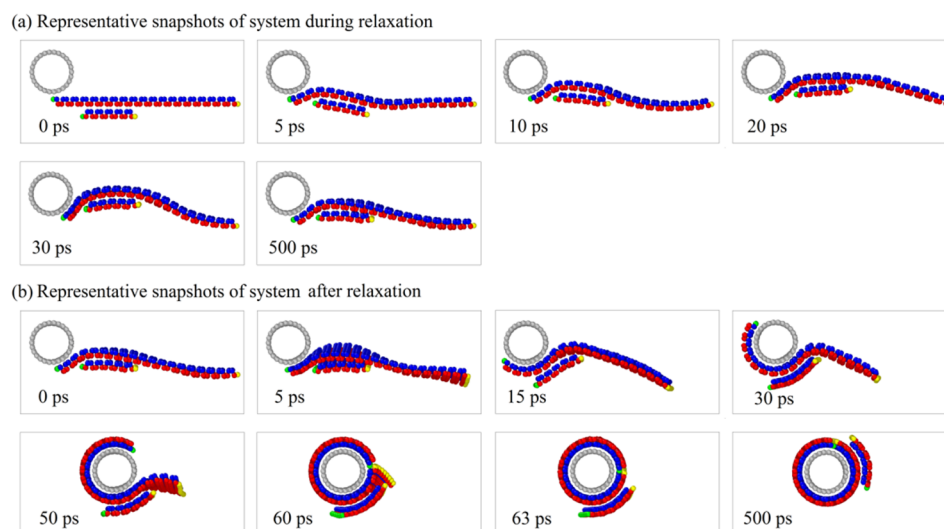


Figure 2. System configurations with $N = 3$ (a) during relaxation and (b) after relaxation. The initial configuration in panel b is identical to the final one in panel a.

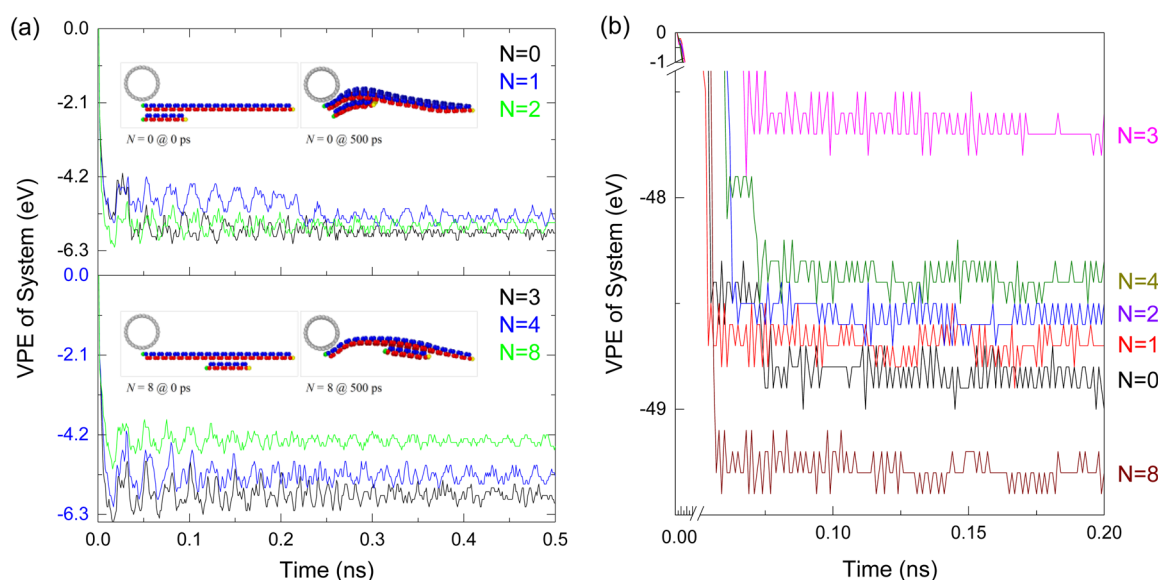


Figure 3. Variation of potential energy of the outside-jammed system with different N : (a) during relaxation and (b) after relaxation and release BP1. The final stable value of VPE in relaxation in panel a is the initial value of that after relaxation in panel b.

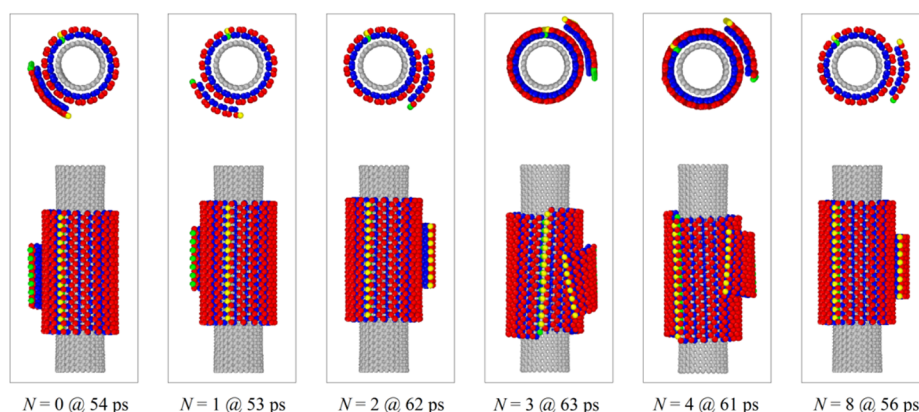


Figure 4. BP nanotubes from BP1 using different winding time and N . The perfect BP nanotube can be formed when $N = 0, 1, 2$, or 8 . If $N = 3$ or 4 , then a chiral BP nanotube is formed.

appearance of each new P–P bond leads to a drop of ~ 0.66 eV potential energy.

3. NUMERICAL RESULTS AND DISCUSSION

3.1. Configuration of Outside-Jammed System with Different Value of N . To discuss the self-assembling process of a nanosystem shown in Figure 1a, that is, the shorter BP ribbon is at the side of BP1 different from CNT, we illustrate the variation of configuration and VPE of the system during relaxation and after relaxation, respectively. In Figure 2a, there are six representative configurations of the system with $N = 3$. Because the right end of BP1 is fixed and the left end can move freely during relaxation, the strong attraction of CNT on the BP ribbon leads to the variation of its configuration. During this period, the value of VPE of system shown in Figure 3a also decreases and tends to be stable after ~ 20 ps. It implies that the configuration of a nanotube system also tends to be stable at the same time. Actually, the fluctuation of a VPE curve (in Figure 3a) reflects the vibration of the middle part of BP1 (see Movie 1), which can be revealed by comparing the configurations during [5, 500] ps in Figure 2a.

Having checked the VPE curves shown in Figure 3a, the system with $N = 8$ was found to be in the lowest decrease rate of VPE among all six cases during relaxation. The reason is that the initial value of potential energy of the system with $N = 8$ is smaller than those with smaller value of N . As N becomes smaller, for example, $N = 0, 1$, or 2 , the interaction among the unsaturated phosphorus atoms at the edges of both ribbons is stronger, which implies larger potential energy of such initial system. After starting relaxation, the relative position of BP ribbons corresponding to CNT can be changed to reduce the potential energy of the system. In particular, BP1 is under tension by CNT. Hence, during relaxation the major part of VPE of the system is caused by the variation of P_1 and P_{C-1} . By comparison of the inserted configurations in Figures 3a and 2a, the curved BP1 has different stable configuration when N is different because the attraction between BP1 and BP2 leads to a small deformation of the area on BP1 overlapped BP2.

After relaxation, BP1 is quickly wound on CNT as its right end is released (see Movie 2). Figure 2b shows some representative configuration of the system when BP1 is wound on CNT. The BP nanotube is formed only requiring 63 ps when $N = 3$. Because of the generation of new P–P

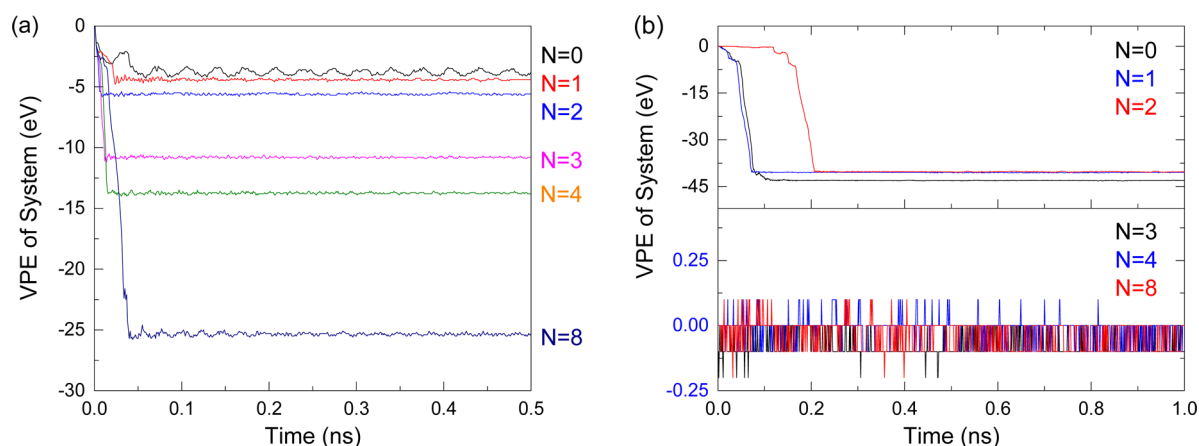


Figure 5. Variation of potential energy of an inside-jammed system with different N : (a) during relaxation and (b) after relaxation and release BP1. The final stable value of VPE in relaxation in panel a is the initial value of that after relaxation in panel b.

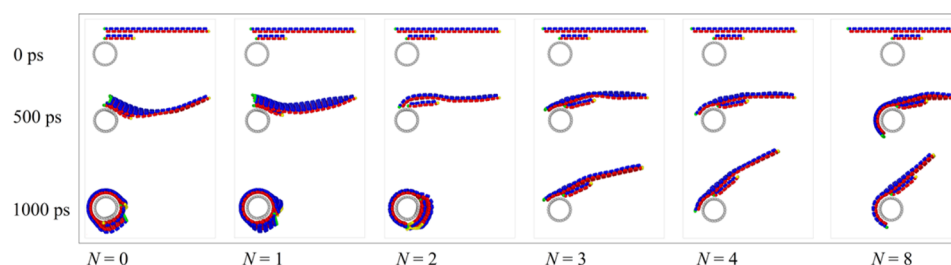


Figure 6. Initial and final system configurations with different N . The snapshots at 0 and 500 ps are obtained during relaxation. The snapshots with respect to 1000 ps are those obtained at 500 ps after the end of relaxation.

bonds in BP1, the potential energy of the system drops further. From Figure 3b, one can find that the potential energy of the system has a drop of ~ 48 eV. For different system with different N , the drop of potential energy of the system is different. For instance, the potential energy of the system with $N = 3$ drops ~ 47.6 eV, while the decrease is ~ 49.3 eV for the system with $N = 8$. The sequence of six final stable values of VPE of the system is shown in Figure 3b. Clearly, the VPE of the system with $N = 4$ decreases faster than that with $N = 3$ only. A justifiable reason is necessary to demonstrate such disorder of the results.

Figure 4 illustrates the BP nanotubes generated from BP1 with different value of N . It can be found that the BP nanotubes are formed in ~ 60 ps when the right end of BP1 is released. However, not all of the BP nanotubes are perfectly formed. For example, when $N = 3$ or 4, the final BP nanotube is a chiral one rather than an armchair nanotube when $N = 0, 1, 2$, or 8. In the chiral BP nanotubes, one can find that not all unsaturated phosphorus atoms at the edges of BP1 are covalently bonded. In this situation, the decrease in potential energy of the system is not as fast as those systems with an armchair BP nanotube. This is the reason why the VPE values of the system with $N = 3$ or 4 decrease slower than those of the rest of the cases. Comparing the system with $N = 3$ to that with $N = 4$ in Figure 4, it can be found that the relative position of BP2 corresponding to BP1 varies differently. When $N = 3$, BP2 has an obvious rotation on BP1. The rotation is smaller when $N = 4$. As rotation displacement happens, the potential energy of a system increases due to the distance between the two BP ribbons increasing. This is the reason why the VPE of the system with $N = 3$ has a slower decreasing rate than that of the system with $N = 4$. The slight difference among the final stable

values of VPE of the systems with $N = 0, 1$, and 2 is attributed to following two reasons. One is that the interaction between the edges of the two BP ribbons changes from being controlled by S–W potential to being controlled by L–J potential before and after forming the perfect BP nanotubes. The other is due to the relative translational motion of BP2 on BP1 along the z direction.

From Figure 4, one can also find the asymmetric geometry of the final system, although the initial configuration shows symmetric geometry as in Figure 1. The reason is that the atoms in the system have thermal vibration. At a canonical NVT ensemble with $T = 8$ K, the temperature is controlled by the Nosé–Hoover thermostat. Hence, velocity of atoms needs to be modified in simulation to satisfy Gaussian distribution. Because of the modification on velocities of atoms, the geometry of the system becomes asymmetric step by step. Because the system configuration is far away from symmetry, relative motion between two BP ribbons becomes more obvious, which can be observed from the results shown in Figure 4.

On the basis of the discussion above, a conclusion is made; that is, as BP2 and CNT are on opposite sides of BP1, the final BP nanotube may not be perfect due to the relative motion (translation or rotation) of BP2 on BP1 during winding process.

3.2. Configuration of Inside-Jammed System with Different Value of N . When the short BP ribbon is closer to CNT, the winding process of BP1 may be significantly different from that of the system with BP1 closer to CNT. The reason is that the short ribbon will reduce the attraction between BP1 and CNT. Under this condition, the amount of potential energy of BP1 could be larger than that of the L–J potential

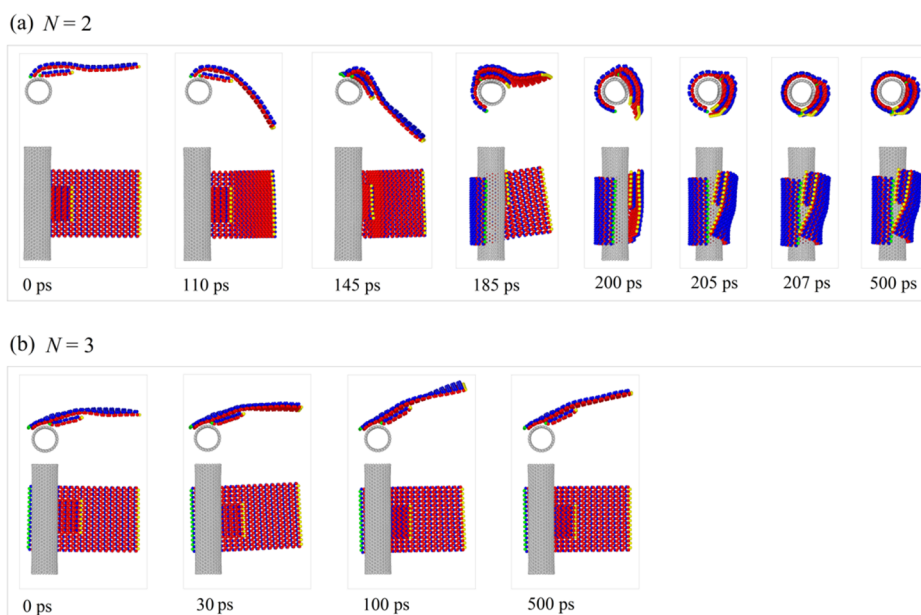


Figure 7. Some representative system configurations with (a) $N = 2$ or (b) $N = 3$ after releasing the right end of BP1.

energy with respect to the attraction of CNT to BP1. Hence, the relative position of BP2, BP1 and CNT is important to the self-assembling process of the nanosystem. When a system has enough relaxation time (e.g., 500 ps relaxation), the final system configuration could be obviously different as compared with its initial configuration. The discussion of the behavior of a system during and after relaxation is presented, separately.

In Figure 5a, the histories of VPE of the inside-jammed system with different N are shown. The VPE of the system with $N = 0$ has the smallest drop. When N increases, the VPE of the system has a significant decrease. In particular, when $N = 3, 4$, or 8, the variation of VPE is >10 eV. This indicates that the system configuration should have an obvious variation during relaxation. On the contrary, in Figure 5b, the VPE of the system with $N \leq 2$ has a heavy decrease, for example, more than 38 eV of drop at ~ 200 ps after the end of relaxation. At the same time, the VPE has slight fluctuation near 0 eV of the system with $N \geq 3$. It implies that the system configuration with $N \geq 3$ has no variation after relaxation. To verify this prediction, we present each system configuration at 0, 500, and 1000 ps in Figure 6. It can be found that BP1 has obvious deformation at its middle part when $N = 0$ or 1 ($N = 0$ or 1@500 ps). The reason is that the attraction between both BP ribbons is stronger than that between BP2 and CNT. The left end of BP1 has no chance to get closer to CNT due to the existence of BP2 between them. When $N = 2$, the left end is attracted on the CNT (see Movie 3). However, the overlap area between BP1 and CNT is very small ($N = 2$ @500 ps) and so is the variation of VPE of system mainly caused by the deformation at the left end of BP1. If N is larger than 2, then the overlap area between the left end of BP1 and CNT becomes larger during relaxation. Owing to the stronger interaction between both BP ribbons, BP2 has no relative sliding on BP1. Hence, the variation of VPE of system with $N \geq 3$ is mainly caused by the winding of BP1 on CNT (see Movie 4) during relaxation.

After relaxation, we release the right end of BP1. It is interesting to find that the final system configuration is sensitive to N . For example, when $N \leq 2$, both BP ribbons and CNT are attracted to each other ($N = 0, 1, 2$ @1000 ps in Figure 6). This

indicates that BP1 has large deformation during winding upon CNT. Hence, the VPE of the system has a significant drop during the same period. However, the system configuration with $N \geq 3$ has no obvious variation except the relative rotation of BP ribbons on CNT ($N = 3, 4, 8$ @1000 ps in Figure 6). It is known that such relative rotation leads to no variation of VPE of the system, which matches well with the curves shown in Figure 5b. The result verifies the prediction of the variation of VPE of the system with different N .

To enhance our understanding on the sensitivity of the system's final configuration to the value of N , we list some representative snapshots of the systems with $N = 2$ and 3 in Figure 7a,b, respectively. When $N = 2$, both BP ribbons are attracted by and finally wound on CNT. Comparing the configurations, we find that the system configuration has no obvious variation during the first 110 ps. From 145 ps, the relative sliding between the two BP ribbons takes place (see Movie 5). Rapidly, the left end of BP1 is wound on CNT. It improves the relative sliding of BP2 on BP1. Until 200 ps, BP2 has approached the right end of BP1. During the same period, BP2 also slips along the axial direction of CNT. Because of the strong attraction among the edge atoms on both ribbons, BP2 does not move out of BP1 along the axial direction of CNT. At the same time, the left end of BP1 is also very close to the right end of BP1 and BP2. Soon after 200 ps, say at 207 ps, the two ends of BP1 are connected by a new P–P bond, and six new P–P bonds are generated to connect the left end of BP1 and BP2. The results are shown in the heavy drop of VPE of a system (particularly P_1, P_{1-2}). Later, the system configuration changes slightly. Both ribbons rotate slowly on CNT. The VPE of system has no obvious variation after 207 ps (see the curve of $N = 2$ in Figure 5b). The relative sliding between the two BP ribbons is triggered by the attraction between BP1 and CNT; when the attraction is stronger than the “static friction” between the two BP ribbons, the relative sliding between the two BP ribbons starts. The “static friction” between the two BP ribbons is mainly caused by the strong interaction between the unsaturated phosphorus atoms on BP2 and the saturated atoms on BP1. From Movie 5, when BP1 is bending toward CNT,

BP2 is forced to curve ($N = 2$ @ 110, 145 ps in Figure 7a) which leads to weaker interaction between the edge atoms on BP2 and BP1. As sliding continues, the “kinetic friction” between the two BP ribbons becomes lower than the “static friction”. Meanwhile, the attraction between BP1 and CNT is not reduced. Hence, the relative sliding between the two BP ribbons does not stop until the two ends of BP1 meet. It should be mentioned that BP2 has bending deformation during the period of relaxation. Because the curvature angle of BP2 is much less than that of BP1, it can hardly be identified. The reason is that bending deformation depends on both the moment applied and the bending stiffness. Meanwhile, the moment is determined by the force and the dimension involved in bending deformation, and the overlap area of BP1 and BP2 has much larger bending stiffness as compared with a single-layer BP ribbon (e.g., BP1 only). Both factors lead to slight deformation of BP2.

From Figure 7b, we can see that the variation of the system configuration contains two aspects (see Movie 6) when $N = 3$. One is the slight vibration of the right end of BP1. It results in a very small variation of VPE that could be positive (Figure 5b and P_1 in eq 1). The other is the rotation of both BP ribbons on CNT, which has no contribution to the variation of VPE. The system configuration in Figure 7b can be considered as stable state because the left end of BP1 is attracted on CNT tightly. BP2 acts as a support to keep the middle part of BP1 slightly curved. At the same time, the right end of BP1 is far away from CNT. Hence, there is no interaction between the right end of BP1 and CNT. This is the why BP1 cannot be wound on CNT and keeps the configuration shown in Figure 7b. Owing to a small friction between CNT and the two BP ribbons, the ribbons can rotate slowly on CNT. It can be predicted that the rotation will stop after a long period of time. Compared with the winding process of BP1 in the system with $N = 2$, it can be predicted that the BP1 with $N = 3$ can also be wound on CNT on the condition that the right end of BP1 has enough velocity toward CNT after being released.

In brief, when BP2 is laid out between BP1 and CNT, BP1 cannot be wound on CNT to form a perfect or chiral BP nanotube.

4. CONCLUSIONS

Because it is difficult to obtain a nanotube from black phosphorene by synthesizing method, we suggest an approach to fabricate it from a BP nanoribbon. By numerical experiments, the approach is validated from the self-assembling results of a jammed BP ribbon on a fixed CNT. On the basis of the discussions above, two concluding remarks are made here for the future design of such 1D material.

(1) When a longer BP ribbon (BP1) is placed nearby a CNT and a shorter BP ribbon (BP2) is at opposite side of BP1, a BP nanotube can be formed from BP1. The chirality of the BP nanotube depends on the initial relative position of BP2 to BP1. The relative motion, especially rotation, of BP2 to BP1 usually leads to a chiral BP nanotube because the end of BP1 near BP2 has obvious vibration along the axis of CNT.

(2) When BP2 is put between BP1 and CNT, we cannot obtain a BP nanotube for whatever the initial relative position of BP2 to BP1. If the adjacent ends (along CNT axis) of BP1 and BP2 are very close, then BP1 can be attracted by and wound on CNT. If BP2 is nearby the middle part of BP1, then the free end of BP1 will be wound on CNT and the fixed end will keep away from CNT even if it is released.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpcc.7b02279.

Movie 1: Outside- $N = 3$ -Relaxation during [0, 150] ps (AVI)

Movie 2: Outside- $N = 3$ -After relaxation during [0, 100] ps (AVI)

Movie 3: Inside- $N = 2$ -Relaxation during [0, 150] ps (AVI)

Movie 4: Inside- $N = 8$ -Relaxation during [0, 150] ps (AVI)

Movie 5: Inside- $N = 2$ -After relaxation during [0, 250] ps (AVI)

Movie 6: Inside- $N = 3$ -After relaxation during [0, 250] ps (AVI)

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Notes

The authors declare no competing financial interest.

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