Formation of single carbon chain bridging two SWCNTs via tensile deformation of nanobud junction

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ARTICLE INFO

ABSTRACT

Molecular junctions formed by a single carbon chain (SCC) bridging two SWCNTs are highly desirable for molecular electronic nanodevices; however, the fabrication is still quite challenging. In this study, we present a novel method to produce a SCC bridging the outer wall of two SWNTs. By separating the carbon nanotube embedding nanobuds junction, carbon atom chain including a few tens of atoms or even up to 100 carbon atoms bridging two SWNTs can be formed. Moreover, we find that embedding nanobuds junction shows extraordinary room temperature superplasticity. The laddering effect, in which the atom chain can be continuously pulled out from the fullerene molecule in the nanobuds junction under tensile loading, is exhibited in this work.

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1. Introduction

Molecular junctions formed by a single carbon atom chain (SCC) bridging two SWNTs are highly desirable and have been considered to be an attractive solution for the fabrication of metal–semiconductor junctions in the design of nanoelectronic devices [1]. Meanwhile, SCC has been regarded as ideal one-dimensional conductor and is perhaps the thinnest interconnection in an ultimate nano-device. Hence SCCs may be applied to future devices such as transport channels, on-chip interconnects for molecular electronic, and spintronic nanodevices. The existence of pure SCCs has been proved by experimental observation [1–7] and measurements [8–13], and transport [12–20] and mechanical prosperities [21–22] and the formation mechanism [23,24] of SCCs have attracted much attention recently; however, synthesizing these unstable objects are still very difficult. In recent years, many studies have been performed to investigate methods of synthesizing SCCs. The proposed techniques include unraveling a nanotube [8,13] or shrinking carbon nanotube [2,4,9], forming SCC inside a carbon nanotube [5,12], deriving carbon atomic chains from graphene or ultra-narrow graphene nanoribbons [3,6,7], and coalescence of functionalized fullerenes filled into a single-wall carbon nanotube [1]. However, these methods are not best suited for large scale production of SCCs and do not lead to controllable junctions. Moreover, even though SCCs can be produced, how to make them into carbon nanotube interconnects is still quite challenging.

In this paper, we show that SCCs can be derived from carbon nanotube nanobuds junction, that is, to form a molecular junction by a single carbon chain bridging two SWNTs naturally. Moreover, the superplasticity of the nanobuds junction and the interesting unwinding cocoons phenomenon in the tensile process is also exhibited.

2. Deriving carbon chains from nanobuds junction

Following the intensive studies of carbon nanotubes and graphene [25–30], hybrid carbon nanostructures have attracted much attention in recent years [31–36]. As a typical carbon hybrid nanostructure, carbon nanotube nanobud is formed by fusing fullerenes and CNTs. In our early study, we have reported that SWCNTs can be welded together via nanobuds (independent of their diameters) even at a temperature below 1500 K, and thus form a new type of carbon nanotube junction, named carbon nanotube nanobuds junction [36].

Molecular dynamics (MD) simulations are conducted to simulate the separating process of two SWCNTs with nanobuds junction. CNT nanobuds have two kinds of structural configurations: (1) attaching configuration, where a perfect fullerene attaches onto the outer wall of a CNT; (2) embedding configuration, where an imperfect fullerene embeds within a carbon nanotube, whose structure is actually imperfect [37]. To facilitate the rest of the discussion, the heat welded nanobuds junction formed by nanobuds with embedding configuration is called embedding nanobuds junction, and the heat welded nanobuds junction

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formed by nanobuds with attaching configuration is called attaching nanobuds junction. Then we will investigate the separating process of the embedding nanobuds junction.

For highly distorted bonds and configurations, the application of empirical interatomic potential becomes an extrapolation and the results have to be treated with caution [38]. In fact, Tersoff–Brenner potential [39,40], Brenner potential [40,41] and its extention [42] have been used widely to study the mechanical behavior of various highly deformed carbon nanostructures [43–47]. Here the second-generation Brenner potential [41] coupled with the Lennard–Jones potential, is employed in our MD simulations. All MD simulations in this study are performed using the code LAMMPS (Large-scaleAtomic/Molecular Massively Parallel Simulator) [48]. It should be noted that the Brenner potential has been used in the earlier MD investigations of SCCs unraveling in both carbon nanotubes and graphene [38,49], which has been supported by experimental results [3,8,9].

The strain rate and the simulation schemes are considered as follows. First, the optimal 'Scheme 2' (S2) as described in Ref. [50] is used in the MD simulation of the loading process, which has been demonstrated to be reliable in MD simulation of carbon nanotubes. In each MD simulation, as shown in Fig. 1(a), the atoms of the upper half of the upper SWCNT and the lower half of the lower SWCNT were held rigid, and all atoms except the boundary ones rigidly held are treated as thermostat atoms. Second, each displacement step is set to be 0.0025 Å and is followed by 1000 relaxation steps, and simulation time step is set to be 0.5 fs, thus the strain rate is in the range from $1.25 \times 10^8 \, \mathrm{s}^{-1}$ to $2 \times 10^8 \, \mathrm{s}^{-1}$ which is in agreement with the reasonable strain rate selected in Ref. [47], and the elongation speed is 0.5 m/s, which is much less than the speed of sound. The length of the open SWCNT (10, 10) and SWCNT (26, 0) are about 4.9 nm (20 axial period length) and 5.1 nm (12 axial period length), respectively; and the wall thickness of a SWCNT is taken as 3.4 Å [51,52].

The per-atom stress tensor for each individual carbon atom α in the system is calculated by the equation [48,53,54],

$$\sigma_{ij}^{\alpha} = \frac{1}{\Omega^{\alpha}} \left(\frac{1}{2} m^{\alpha} v_i^{\alpha} v_j^{\alpha} + \sum_{\beta=1,n} r_{\alpha\beta}^j f_{\alpha\beta}^i \right) \tag{1}$$

Where α and β are the atomic indices, Ω^{α} represents the volume occupied by atom α, i and j denote indices in the Cartesian coordinate system, m^{α} and v^{α}a denote the mass and velocity of atom α, $r_{\alpha\beta}$ is the distance between atom a and b. The global stress is calculated by averaging over all carbon atoms in the system. The volume of the monoatomistic carbon chain is calculated by $V = \frac{1}{4}\pi d^2 L$, where d and L are the diameter and the length of the chain, and d is set as 3.35 Å.

Taking the SWCNT embedding nanobuds junctions as an example, an interesting unwinding cocoons phenomenon can be observed when separating the SWCNTs (26, 0) nanobuds junction. Atom chain can be continually pulled out from the fullerene molecules, and the fullerene molecules in the nanobuds become smaller and smaller, just like the process of unwinding silk thread from silkworm cocoons, as shown in Fig. 1 and Video 1. This process is different from the processes obtaining the SCC from nanotube or graphene hitherto reported which resembles unraveling the sleeve of a sweater or sweater pieces.

The production of single carbon chains and the formation of junctions by single carbon chains have been quite challenging, however, it can be observed in our simulation that, by the laddering effect exhibited in the tensile process of a SWCNT nanobuds junction, single carbon atom chains consisting of a few tens of atoms or even up to 100 carbon atoms can be obtained. In summary, we have provided a new way to produce single carbon chains and carbon chain bridging carbon nanotubes.

The typical tensile stress versus displacement relationships are shown in Fig. 2 for SWCNT (10, 10) and SWCNT (26, 0) embedding nanobuds junctions, respectively. It is clear that all the stress-strain curves have four distinct stages. Take SWCNT (26, 0) embedding nanobuds junctions as an example, Stage 1 is the initial linear region where elastic elongation controlled by altering the C—C bond angles occurs in the nanobuds junction. In Stage 2, bond breaking and reconstruction occurs in the heat welded fullerene molecular in the nanobuds junction; however single carbon atom chain has not appeared. In Stage 3, monoatomic chain grows and atoms are continually pulled out from the fullerene molecules. As shown in Fig. 2, the separating displacement of SWCNT (10, 10) and SWCNT (26, 0) nanobuds junctions formed by the nanobuds with embedding configuration can reach
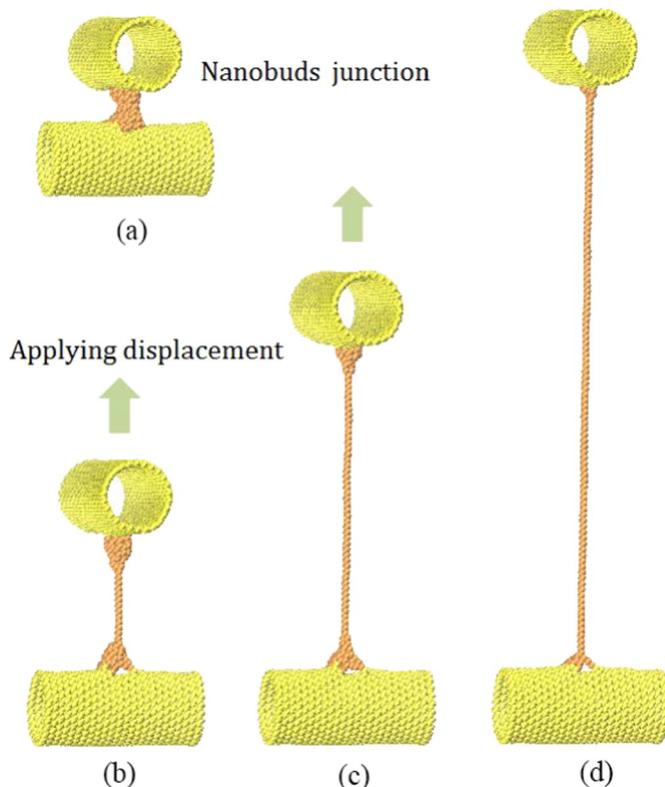

Fig. 1. Typical laddering effect exhibits in separating process of a SWCNT embedding nanobuds junction and the formed long carbon atom chain bridging two SWCNTs.
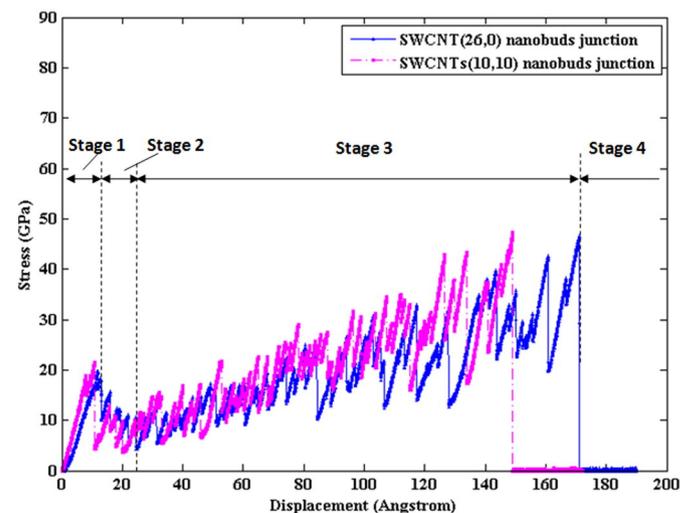

Fig. 2. Tensile stress versus displacement relationships for SWCNT (26, 0) and SWCNT (10, 10) nanobuds junctions when separating the two SWCNTs.

149.1 Å and 171 Å, which corresponds to the maximum elongation 573.6% and 551.6%, respectively. It should be noted that the tensile stress value in Fig. 2 is the mean tensile stress of the system except the region held rigid. In Stage 3, the increased stress mainly comes from stretching the bond length of atom chain. Moreover, the force in the separating process of SWCNT (10, 10) nanobuds junctions is calculated and shown in Fig. 3. It can be observed that though the maximum tensile stress value appears at the point of the atom chain breaking, the maximum force of the system actually appears at the end of the Stage 1.

Due to the time scale limitation of MD simulations, the strain rate has to be set relatively high compared to experiments. Strain rates ranging from 2×10^8/s to 4×10^9/s are investigated, as shown in Fig. 4. We find that the characters of stress variation at different strain rate are similar. Although the maximum strains of the simulations are different, the maximum strains obtained at strain rate 2×10^8/s and 4×10^8/s are very close, thus the strain rates we choose in the simulations ranging from $1.25 \times 10^8\,s^{-1}$ to $2 \times 10^8\,s^{-1}$ are reasonable. In addition, randomness can be observed in the simulation. Some atoms in the tube at the nanobuds junction area sometimes are pulled into the chain, which thus makes the overall stress larger.

Superplasticity can be loosely defined as the ability of a crystalline material to undergo tremendous elongations prior to failure, on the order of hundreds or thousands of percent. Reports have shown that at high temperatures individual single-walled carbon nanotubes can undergo superplastic deformation and attain nearly 280% longer in strain [55]. From the results obtained above, conclusion can be obtained that SWCNT embedding nanobuds junctions can have extraordinary room temperature superplasticity as well.

The energy variation in the process of deriving carbon chains from SWCNT embedding nanobuds junction are analyzed, as shown in Fig. 5, which corresponds to the tensile stress versus displacement relationships of SWCNT (26, 0) nanobuds junctions in Fig. 2. When atoms in the fullerene molecules are pulled out, the bond break releases energy which is absorbed by the system. In Stages 2 and 3, each rapid energy release associated with an irreversible bond breaking process arises a pulse type kinetic energy change for both C_{60} and the SWCNTs in the nanobuds junction. The single carbon atom chain break result in the maximum kinetic energy variation for both the carbon nanotube and the heat welded fullerene molecules in the nanobuds junction, as shown in Fig. 5(a) and (b). This pulse type kinetic energy change result from the bond breaking should have important influence in the growth of the single carbon atom chain. When separating multiple nanobuds junction between two SWCNTs, the incompatibility of the pulse type kinetic energy change created by each single atom chain is disadvantageous for the growth of the atom chains, and the failure or the energy
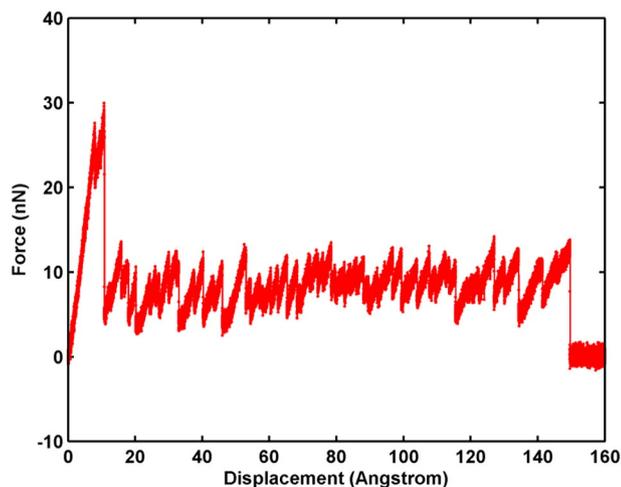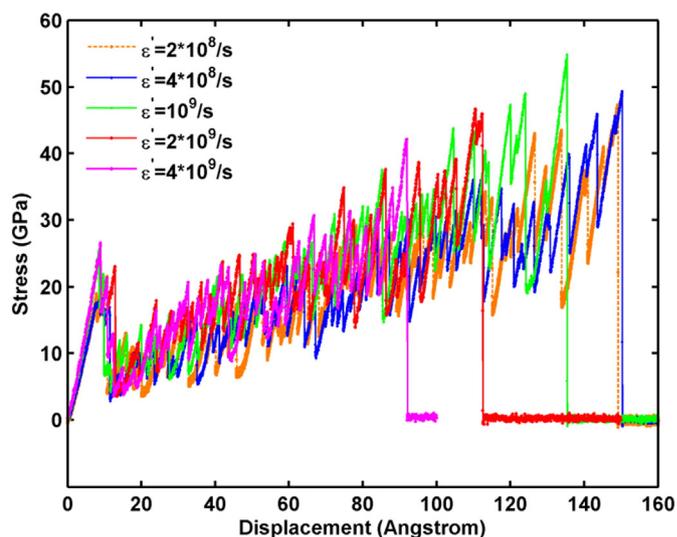

Fig. 4. Effect of different strain rates on the deformation behavior of a SWCNT (10, 10) nanobuds junctions when separating the two SWCNTs.
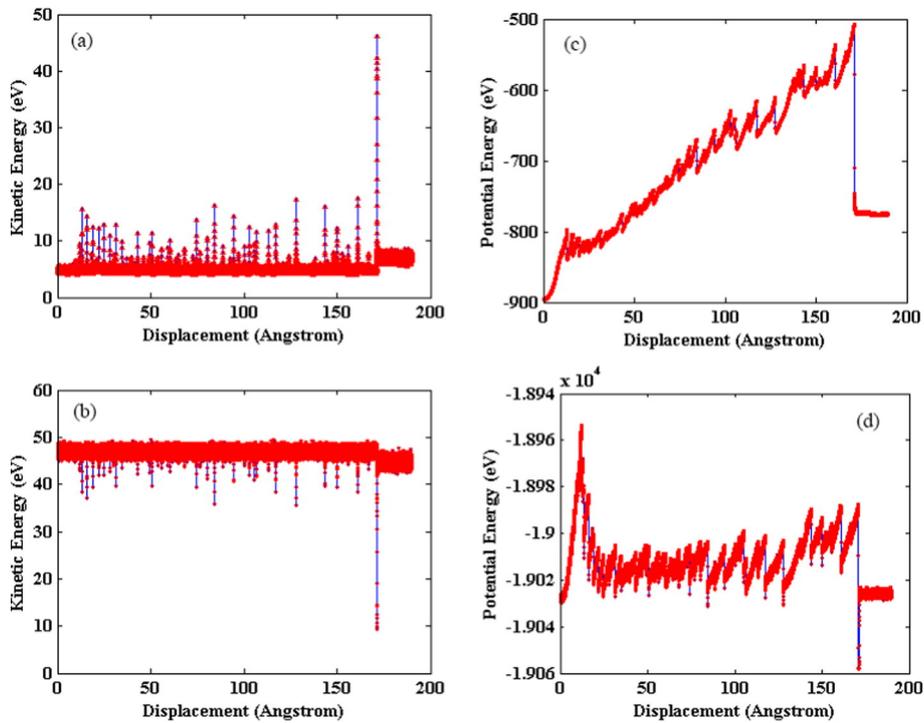
change of one of the chains will affect other chains, and thus long multiple freestanding carbon atoms chains cannot easily survived.

As shown in Fig. 5(c), the overall potential energy of fullerene molecules in the nanobuds junction increases with more and more atoms pulled out from the heat welded fullerene molecules, which corresponds to the overall stress increase of the system in Stage 3. As shown in Fig. 5(d), it can be observed that the potential energy change is very small in Stage 3 except its final period, in which plastic deformation occurs at the tube in the junction area, and one or two atoms on the carbon nanotube are pulled into the junction region.

A stable carbon chain bridging carbon nanotubes is potentially attractive as a molecular electronic device [1]. To test the stability of the carbon atom chain obtained by separating the nanobuds junction, the atom chains are unloaded at temperature of 300 K before it is broken. For example, three typical models A, B, and C are chosen, where model A with a length 168.86 Å is single carbon atom chain before unloading, and models B and C are obtained by unloading the carbon atom chain shown in Fig. 1(d) to 136.69 Å and 110.37 Å, respectively, as shown in Fig. 6. Though the carbon atom chains shake seriously in the unloading process, it is very stable except Chain C, in which reconstruction occurs at the ends, and two atoms are pulled into the single atom chain from the rest of the fullerene molecules attached to SWCNT. In Fig. 6 (D1, D2), the bond id is indicated, with $n = 100, 100$ and 102 for the single atom chains models A, B and C, respectively.

Another important issue is the stability of the single carbon atom chain. In Ref. [1], the short SCC bridging the two SWNTs within a host tube is stable up to a temperature of 1000 K. To test the stability of the long single carbon atom chain formed by separating the nanobuds junction in our work, the systems of the molecular junctions formed by a single carbon chain bridging two SWNTs are heated from 300 K up to 2000 K in 400 ps with a fixed timestep 0.1 fs using the Nosé–Hoover thermostat for the above models A, B and C. Results show that the single carbon atom chain models A, B and C are stable up to temperature limits of 500 K, 1900 K and 2000 K, respectively. For Model A, when temperature is higher than the limits, the chain often breaks; however, for models B and C, the attachment point of the chain to the rest of fullerene moves and reconstruction of the rest of fullerene occurs, which forms a longer single atom chain and finally disconnects from the SWCNT.

To understand the bond length variation of the SCC at different temperature, the systems of the molecular junctions formed by a single carbon chain bridging two SWNTs are equilibrated for each model at 300 K, which is held constant for 100 ps with a fixed timestep 0.1 fs using the


Fig. 3. Tensile force versus displacement relationships for SWCNT (10, 10) nanobuds junctions when separating the two SWCNTs.

Fig. 5. Typical energy variation in nanobuds in the separating process of SWCNT (26,0) nanobuds junction: (a) kinetic energy variation of C_{60}s in the nanobuds junction; (b) kinetic energy variation of SWCNTs in the nanobuds junction; (c) potential energy variation of C_{60}s in the nanobuds junction; (d) potential energy variation of SWCNTs in the nanobuds junction;

Nosé–Hoover thermostat. The bonds lengths of the SCCS at different temperature are shown in Fig. 7. It is shown that the magnitude of the bond length alternation is independent of the temperature, which is in agreement with the results in Ref. [1] for the short SCC bridging the two SWNTs within a host tube. However, it is obvious that the bond length alternation is related with the stress applying on the molecular junctions via single carbon chain bridging two SWNTs. It can be seen from the Fig. 7 that for model B and C obtained by unloading, the bond lengths at the anchor with bond id = 1, 2, n − 1 and n is larger than the bonds in the single carbon atom chain. However, in model A,

the bond lengths in the atom chain and the anchor points in the rest of fullerene molecules attaching on the SWCNTs is very close. This can explain why the chains of model A break at the middle but the chains of models B and C do not when temperature is higher than the limits.

Moreover, in Fig. 7, the calculated average forces applying on the chain A, B and C are 9.7 nN, 1.2 nN and 0 nN at temperature of 300 K, and the equilibrated bond length of SCC is about 1.33 Å at 300 K, which is consistent with that in Ref. [23], and the bond length of the SCCs ranging from 1.33 to 1.75 Å in Fig. 7 is also consistent with that in Ref. [23] which is 1.33–1.72 Å, however the resulting strain on the
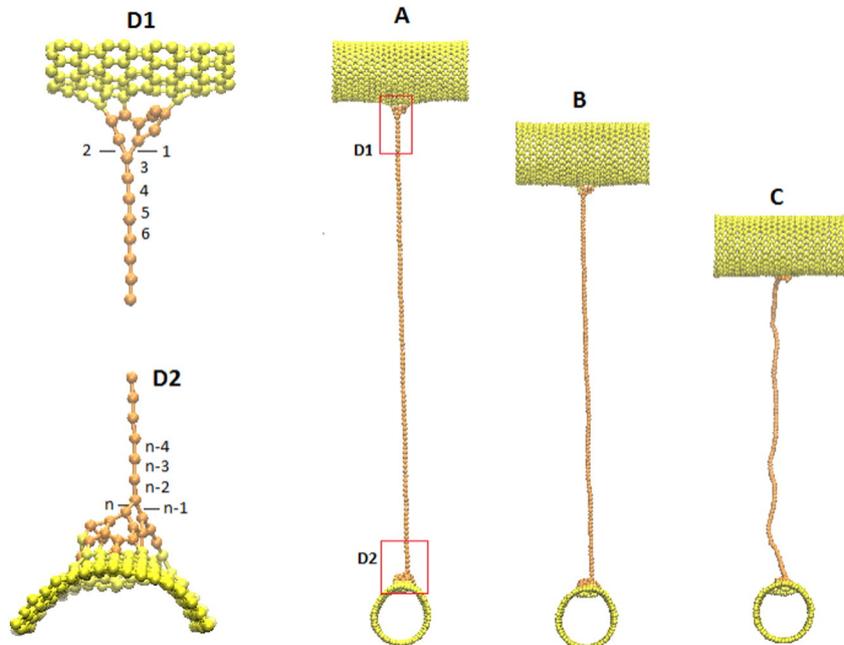
Fig. 6. 3 typical models A, B, C of single atom chain are chosen before or after unloading: (A) Snapshots from simulations at 300 K before unloading with chain length 168.86 Å; (B),(C) Snapshots from simulations at 300 K after unloading with chain length 136.69 and 110.37 Å, respectively; (D1),(D2) the bond numbers indicated.
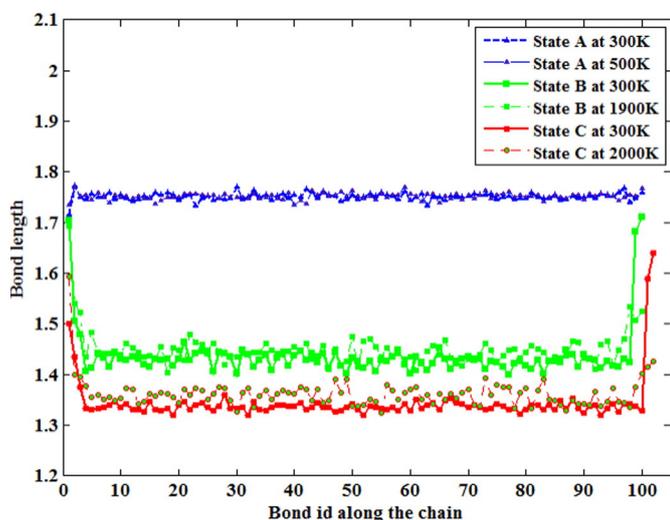
Fig. 7. Bond lengths between the single atoms of the chain taken from snapshots from MD simulations at different temperature.

order of 20% to 30% is larger than those in Refs. [56,57]. We must admit that the bond length of MD simulations cannot exactly agree with those from the first principle. However, as mentioned in Ref. [23], the equilibrated bond length of SCC 1.33 Å is closed to correct bond lengths of cumulene, which is about 1.28 Å.

Theoretically, stable carbon chain structures may be double-bonded (polycumulene), or alternating single-triple bonded (polyyne) [56]. Although the alternating polyyne form has also been shown to be more energetically favorable, cumulenic chains are often produced in conjunction with more complex terminations [1]. Marques et al. [58] reported their work on the formation of SCCs by breaking of carbon nanotubes under tension, and they found the character of the bonds in the linear chain was found to be of cumulene-type, i.e, with all nearly equivalent bond lengths. Ravagnan et al. [59] showed cumulene-type SCC can be formed by sp^2 bonding to graphitic fragments and graphene nanoribbons (NRs), and such cumulene-type SCC displaying a non-negligible bond-length alternation (BLA). They suggested that the traditional categories of polyynes (alternating single-triple bonds, yielding a

large BLA) and cumulenes (double bonds, negligible BLA) appear too simplistic for the description of these systems. In our work, the obtained carbon atom chains are cumulene-type with a small but non-negligible BLA, which are agreement with those in Ref. [58,59].

3. Discussions

For the issue of the formation of molecular junctions by a single carbon chain bridging two SWNTs, one question that arises is if carbon chains can also be derived from the carbon nanotube junction. To test it, a series of MD simulations of separating the two SWCNTs with junction are conducted. Here we take SWCNTs (5, 5) junctions [60] as example. In each MD simulation, the atoms of the upper half of the upper SWCNT and the lower half of the lower SWCNT are held rigid. As shown in Fig. 8, the connected bonds number in junction A, B, and C is in ascending order, thus the junction C is the strongest junction among these junctions.

Tensile stress versus displacement relationships for SWCNT (5,5) junctions when separating the two SWCNTs are shown in Fig. 8. It can be clearly observed that the maximum elongation for SWCNT (5, 5) junction is much less than that of the nanobuds junction. In fact, the carbon atom chains consisted of less than 10 atoms can also be formed in the separating process of SWCNTs junction C in the simulations; however, the SCCs obtained are too short for Junction A and Junction B and the method is not easy to control. Carbons are more apt to be pulled from the system due to the imposed curvature and intrinsic pentagons of the fullerene. As suggested in Ref. [24], the formation of longer chains may be associated with the presence of Stone-Wales defects close to the carbon dimers. However, for tube-tube junction, we find that only short SCCs can be formed even if Stone-Wales defects present in the junction area. This may indicate that SCC is not easily formed by using the tube as a ladder-source in the transverse direction.

In earlier reports, only the C$_{60}$ nanobud and nanobud junctions have been discussed. In fact, other fullerenes beside C$_{60}$, also can attach or be embedded on the outer surface of the CNT to become good welding materials for heat welding of CNTs. Here we take C$_{180}$ as example, as shown in the subfigure of Fig. 9, C$_{180}$ embedding nanobuds junction can be formed by heat welding using the same method [36]. Carbon atom chain and molecular junctions formed by SCC bridging two SWNTs
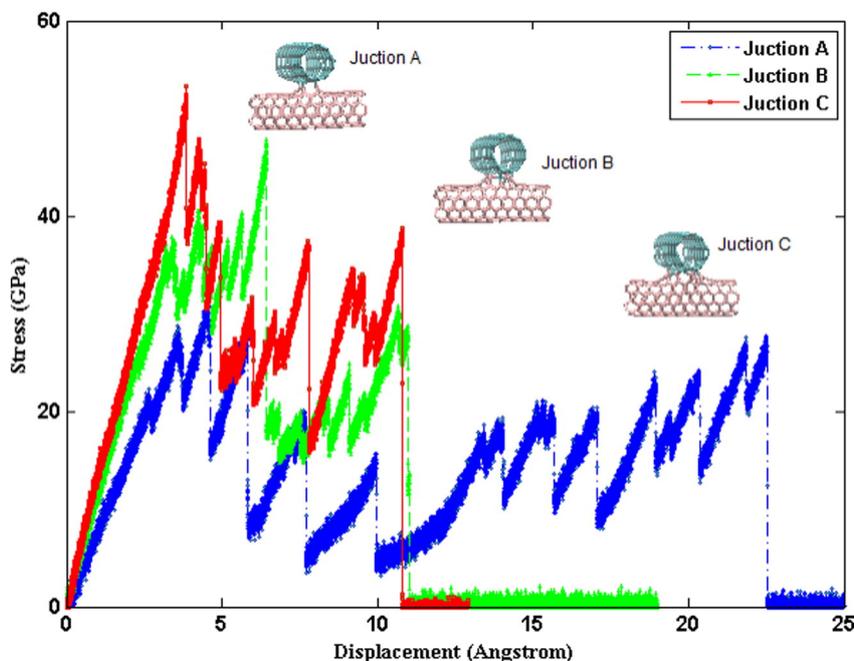

Fig. 8. Tensile stress versus displacement relationships for SWCNT(5,5) junctions when separating the two SWCNTs.
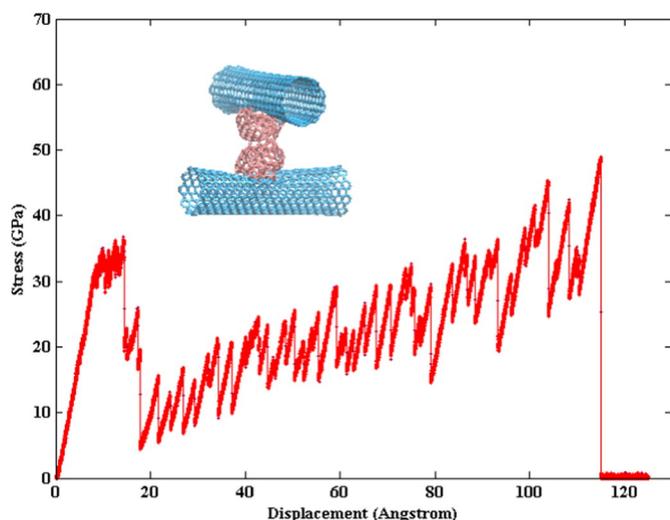
Fig. 9. The separating stress of SWCNT(10,10) nanobuds junction via C_{180} nanobuds.

also can be obtained by separating the C_{180} embedding nanobuds junction.

It should be noted that the nanobuds junction discussed above is the embedding nanobuds junction, and the separating process and the characteristic are different for attaching nanobuds junction. For SWCNT attaching nanobuds junction, the atom chain generally forms between the tube and heat welded fullerene molecules when separating the two SWCNTs, because the strength of the bond connection between the tube and heat welded fullerene molecular is less than the connection between the two heat welded fullerene molecular. Moreover, although sometimes carbon atom chain containing a few tens of atoms also can be obtained when separating the attaching nanobuds junction; however, the formation quite depends on the strength and configuration of the junction area between the tube and the fullerene molecules. If the bond connection between the tube and heat welded nanobuds is not strong enough, no atoms chain forms.

4. Conclusions

We present a method to produce molecular junctions formed by a single carbon chain (SCC) bridging the outer wall of two SWNTs via separating the SWCNTs embedding nanobuds junction. The obtained SCCs can include a few tens of atoms or even up to 100 atoms and have good stability which can be stable up to a temperature of 2000 K. The superplasticity of the nanobuds junction and the interesting unwinding cocoons phenomenon in the tensile process are exhibited in this paper for the first time. When separating the SWCNT nanobuds junction, atom chain can be continually pulled out from the fullerene molecules, and the fullerene molecules in the nanobuds become smaller and smaller, just like the process of unwinding silk thread from silkworm cocoons.

Moreover, the nanobuds junction is also compared with the SWCNT junction, and we find the above unique behavior shown in the nanobuds junction cannot be observed in SWCNT junction. We also demonstrate that fullerene group beside C_{60}, e.g. C_{180} also can form nanobuds and nanobuds junctions, which owns similar behavior as nanobuds junction via C_{60}.

In conclusion, using the simple method proposed in this work, both carbon atom chains consisted of a few tens of atoms or even up to approximately 100 carbon atoms and molecular junctions formed by a SCC bridging two SWNTs can be obtained. From an experimental point of view, this method overcomes the difficulty of transferring carbon wires to substrates and coating metallic electrodes because in this method the carbon nanotube is already on a substrate and can be used as an electrode directly. This opens new exciting possibilities for research studies and applications of carbon atomic chains for molecular electronic nanodevices. However, due to the time scale limitation of MD simulations, the strain rates employed in our work still are relatively high compared to experiments. Moreover, how to form individual embedding nanobuds junction experimentally is still quite challengeable. Therefore, further theoretical and experimental works for the validation of the proposed mechanism will be planned in the future.

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.matdes.2016.02.061.

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