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Tensile Properties of Partially Unzipped Carbon Nanotubes

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Abstract

We have studied the tensile properties of partially unzipped carbon nanotubes. We have found that when the edge dangling bonds are not passivated partially, unzipped carbon nanotubes show diverse structural transformation behaviours at ambient temperatures. The dangling bonds tend to rebond under certain conditions, leading to structure back to the original carbon nanotube pattern and the speed of such self healing increases with rising temperature. When the cutting length is sufficiently large or the diameter of the original tube is small, the unzipped graphene end rolls up and forms various patterns, which is good agreement of previous theoretical and experimental work.

INTRODUCTION

Iigima [1] studied the properties of carbon nanotubes. Kosynkin et al [2] and Kim et al [3] reported results of producing graphene nano ribbons from longitudinal unzipped of carbon nanotubes. The resultant graphene nano ribbons showed the better applications in nano electronic devices. Geim and NOvoselov [4] and Neto et al [5] showed that discovery of graphene had become a good form of carbon materials due to its excellent electronic mechanical and magnetic properties. Li et al [6] and Cai et al [7] Synthesized graphene nanoribbons. Cano et al [8] and Paiva et al [9] studied that unexpected by-product of unzipped structure was found in some experiments. Santos et al[10] and Huang et al [11] showed that such unexpected structures have extra ordinary electronic and magnetic properties. The obtained our results were compared with the previously obtained theoretical and experimental results.

METHOD

It was developed for hydrocarbons on the basis of the Tersoff-Brenner expression and the Lennard-Jones potential in the form of

$$V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right) - \left(\frac{\sigma}{r_{ij}}\right)\right]$$

describing long range Vander Waals interaction, was also included. Lennard-Jones constants used in simulation are $\varepsilon = 51.2K$ and $\sigma = 2.28\text{Å}$. This method has been widely used in studies of carbon nanotubes. It has produced for understanding deformation under various loading conditions, nonlinear elastic scaling behavior and enhanced mechanical properties. It has also proved well in describing bonding-debonding processes of carbon materials. The Berendsen thermal schemes have been employed to control temperature in the simulations. The partially unzipped carbon nanotubes are obtained by longitudinally cutting one row of carbon-carbon bonds and relaxing the structure at near zero temperature.

RESULTS AND DISCUSSION

Fig (1) shows the results for a partially unzipped single walled carbon nanotube where the unzipping length L along the axis direction in this model is 7.4 nano meter. It is seen that at low temperature at 5 K, the partially unzipped single walled carbon nanotubes are stable and the dangling bonds at the cutting edge show no reconstruction as observed in flat graphene nano sheets. When we heat the system to higher temperatures, the edge dangling bonds lose their stability. Reconstruction behavior frequently observed in graphene nano ribbons edges, the unsaturated carbon atoms at the cutting front reconnect to each other and the whole structure thus self heals back to the original carbon nanotubes geometry, because dangling bond states have higher energy. At the junction area between the carbon nanotube and graphene segments, strong local stress exists since the carbon-carbon bond length in the carbon nanotube segment is elongated the carbon-carbon bond length at the cutting crack front. Two driving forces together with thermal energy pull dangling atoms at the edges of the graphene segment backward each other, thus the unzipping front of the partially 3 unzipped carbon nanotube tends to roll back to circular shape at sufficient temperature. We have examined this behavior at a series of temperatures upto 400K, which is shown in fig (1). Graph (1) shows a general decreasing trend of healing rate against cutting length. This behavior is seen for the bending stiffness of the unzipped graphene nano ribbon segment. Due to the different edge state of the graphene nano ribbon segment from that of armchair partially unzipped carbon nanotubes, the healing speed is slightly slower than the corresponding healing behavior and its temperature and cutting length dependence remain similar the tensile deformation behavior of a zigzag partially unzipped carbon nanotube results is shown in graph (2). When tensile strain is applied to the sample, the rippling is effectively suppressed resulting in an ultra flat graphene structure engineering aimed at using ultraflat graphene for exploring true two dimensional physics. We examined the hydrogen saturation effect on tensile behavior of partially unzipped carbon nanotubes. We found that there is no noticeable difference from those of bare edge structure, both the elastic limits and the feature patterns remain the same as obtained previously.

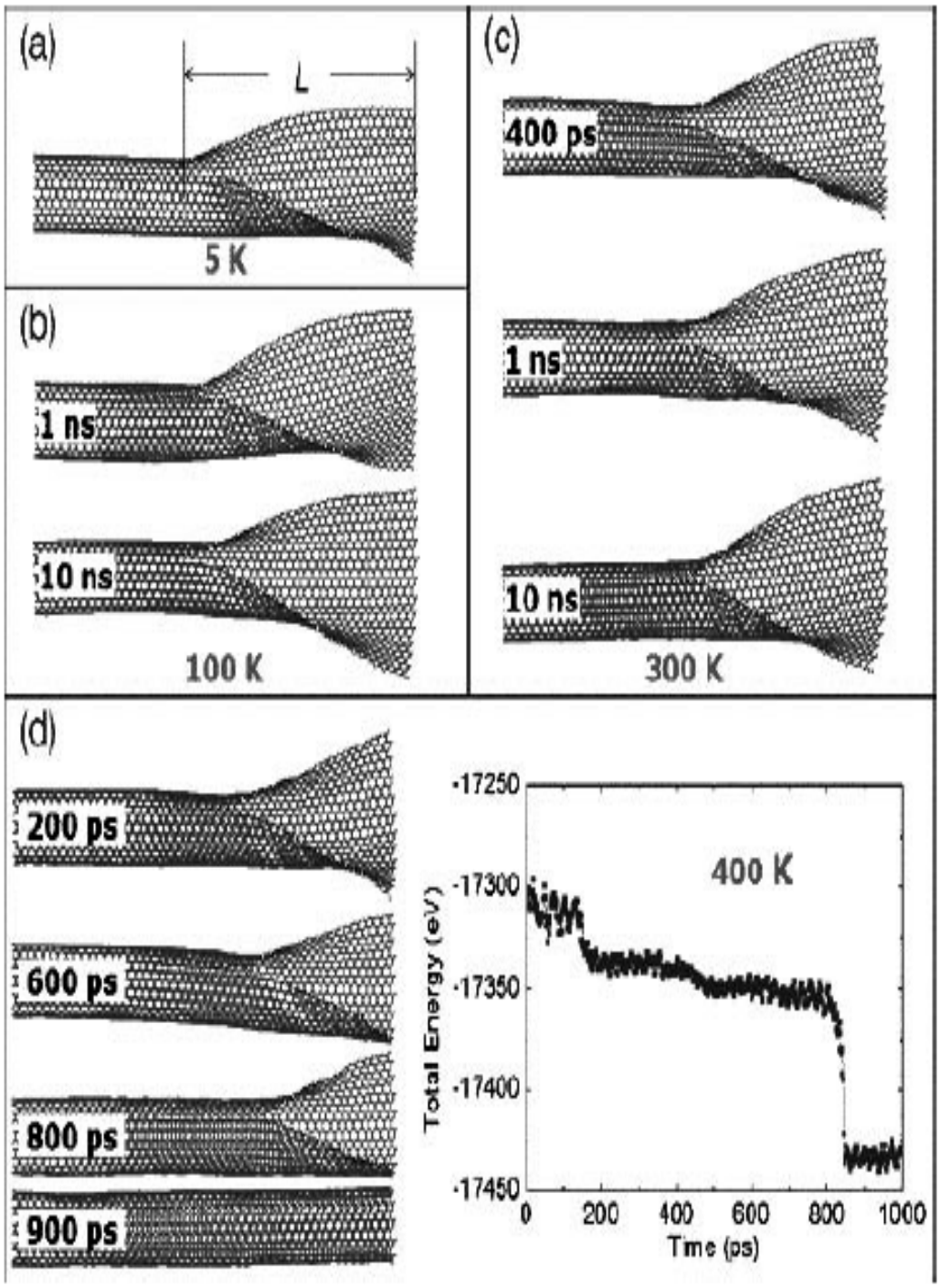
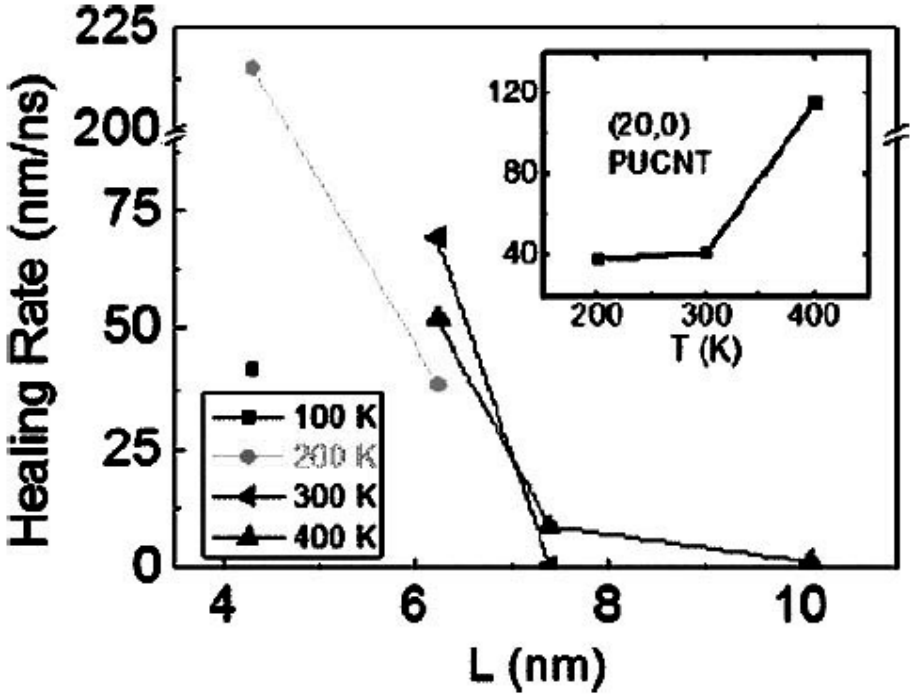
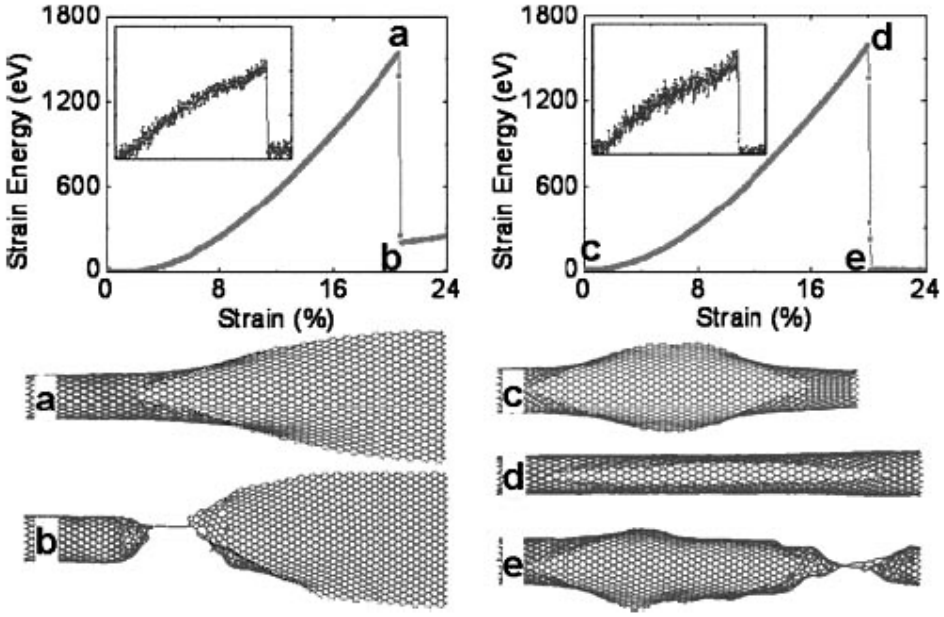


Fig. 1: Partially unzipped CNT relaxed at different temperatures.



Graph 1: Cutting-width-dependent healing rate of a PUCNT. Inset presents the healing rate of a PUCNT vs temperature



Graph 2: Tensile properties of a partially unzipped CNT with different unzipping geometry.

CONCLUSION

We found that in the absence of edge passivation partially unzipped carbon nanotubes are unstable with rising temperatures. The dangling bonds at the cutting front tend to reconnect to each other and form back to carbon nanotube structure. Partially unzipped carbon nanotubes show diverse structural transformation behavior at ambient temperatures. Simulation results showed that partially unzipped carbon nano tubes exhibited brittle fracture mode at room temperature. The snapshots of the structure during stretching demonstrated the brittle fracture pattern. It was seen that the broken sites located at the junction area that linked the carbon nanotube and the graphene nanoribbon segments. We found that in all tensile tests this fracture mode remained universal tensile deformation behavior of zigzag partially unzipped carbon nanotube showed similar patterns for armchair structure. The strain free graphen nanoribbon structures in simulations showed intrinsic ripping behavior with a typical wave length 7.8 nanometer. In the case of graphene edges when they are hydrogen saturated the self healing behavior was suppressed our obtained results were in good agreement with experimental results obtained earlier.

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