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Theoretical analysis on electronic properties of zigzag-type single-walled carbon nanotubes under radial deformation

Yoshitaka Umeno *, Takayuki Kitamura, Akihiro Kushima

Department of Engineering Physics and Mechanics, Graduate School of Engineering, Kyoto University, Yoshida-Hommachi, Sakyo-ku, Kyoto-shi, Kyoto 606-8501, Japan

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Abstract

Carbon nanotubes (CNTs) have been attracting attention because they have characteristic mechanical and electronic properties. It has been reported that single-walled CNTs can induce large deformation without bond breaking. Therefore, it is of interest to elucidate the electronic properties of CNTs under large deformation. We investigate the deformation behavior and the change in the electronic properties of zigzag-type single-walled CNTs with chiral vectors of (8,0), (12,0) and (14,0) under radial compression with semi-empirical band calculations based on the tight-binding method. The resistance against the deformation increases with the deformation, and its behavior depends on the diameter of the CNTs. The CNTs, which have band gap energy at the initial state, become metallic by the compression.

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Keywords: Carbon nanotube; Radial compression; Electronic property; Band gap energy; Deformation; Tight-binding

1. Introduction

Carbon nanotubes (CNTs), which were discovered by Iijima in 1991 [1,2], have been attracting attention for application to electronic nanodevices because of their structural stability and prominent electronic properties. After the electronic structure of CNTs has been studied in detail [3–5], effect of axial deformation has been investigated [6–11] on the basis of simulations. Our group employed numerical simulations to investigate the change in band gap energy under high axial tension for various structures of CNTs, and found the transition between metallic and semiconducting properties under the deformation and its dependence on the chiral structure [11].

However, controlling the electronic property by the axial tension or torsion is somewhat unrealistic because it is very difficult to apply proper

* Corresponding author. Tel./fax: +81-75-753-5256.
E-mail address: umeno@kues.kyoto-u.ac.jp (Y. Umeno).
URL: http://cyber.kues.kyoto-u.ac.jp.

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deformation. On the other hand, the radial compression is easy to control and can be realized by pressing a tube on a substrate for example. In this study, we conduct tight-binding (TB) semi-empirical band calculations to evaluate the change in the electronic properties of zigzag-type single-walled CNTs with chiral vectors of (8,0), (12,0) and (14,0) under the radial compression.

2. Simulation procedure

Simulation models are shown in Fig. 1. The number of atoms and the initial diameter of the models are indicated in the figure. Simulation on the deformation of the CNTs is conducted by the four-orbital TB calculation with the potential proposed by Papaconstantopoulos and Mehl [12]. The validity of the potential on the CNTs has been confirmed [11] by ab initio DFT calculations based on the norm-conserving pseudopotential method [13]. As shown in Fig. 2, the radial compression is applied on the atoms colored in black displacing in the y (and $-y$) direction, while the cell size in the z direction is constraint. The displacement, y_{-}, is increased by Δy_{-}, and at each step the atomic configuration is relaxed by molecular dynamics (MD) calculations [14,15] where the kinetic energy of the atoms is removed every certain steps. Five **k**-points along the z-axis are adopted in the MD calculations. The **k**-point convergence was carefully examined by preliminary calculations. For the evaluation of band structures, which requires more **k** points, 50 points are employed.

3. Results and discussion

3.1. Mechanical behavior

Figs. 3–5 show the relationship between the applied load, P, and the normalized displacement, δ, of the (8,0), (12,0), and (14,0) tubes, respectively. The change in the shape of the tubes is also depicted in the figures. In the case of the (8,0) tube, the load increases with the displacement. The inclination of the curve, which indicates the resistance against the deformation, increases monotonically except the region of small deformation. This is consistent with the deformation in an elastic tube under continuum mechanics—the elasticity is due to the wall of the tube has resistance against bending.

On the other hand, in the cases of the (12,0) and (14,0) tubes, the curves consist of two regions: gentle slope ($\delta < 0.7$) and rapid increase over $\delta = 0.7$. At the first stage, the resistance is caused by the change in the curvature of the sidewall. The

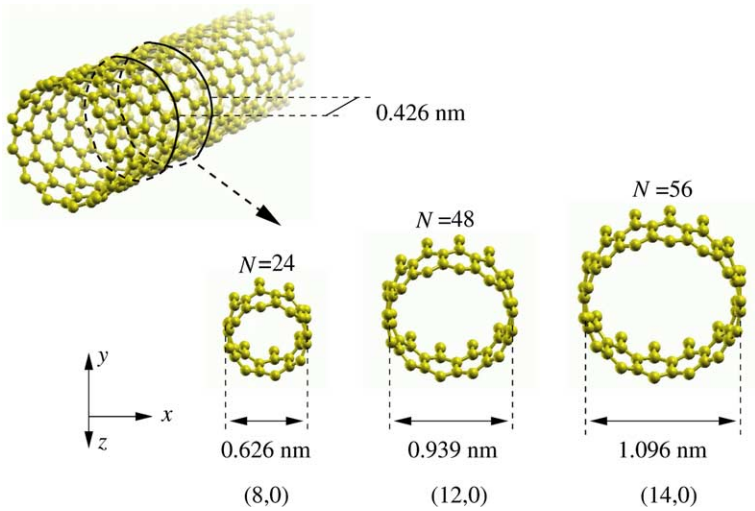

Fig. 1. Simulation models.

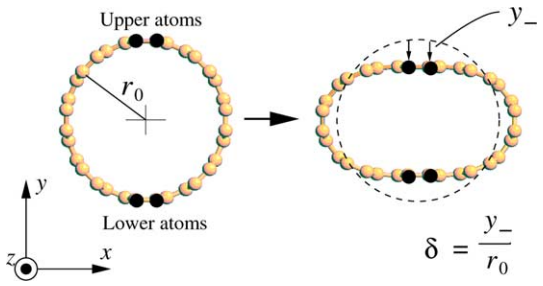

Fig. 2. Radial compression of CNTs.

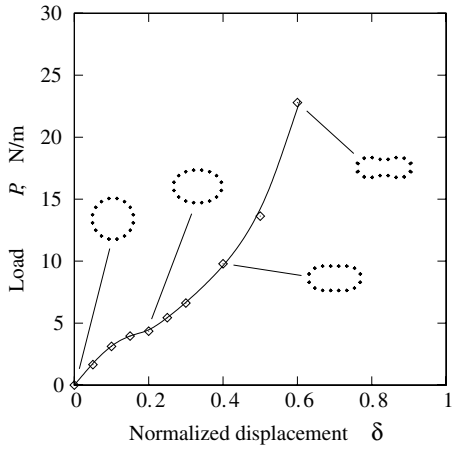

Fig. 3. Change in load of (8,0) CNT under radial compression.

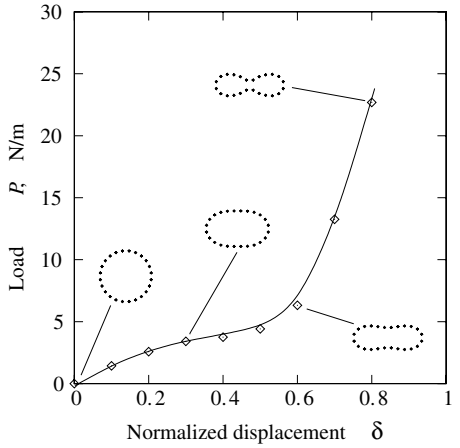

Fig. 4. Change in load of (12,0) CNT under radial compression.

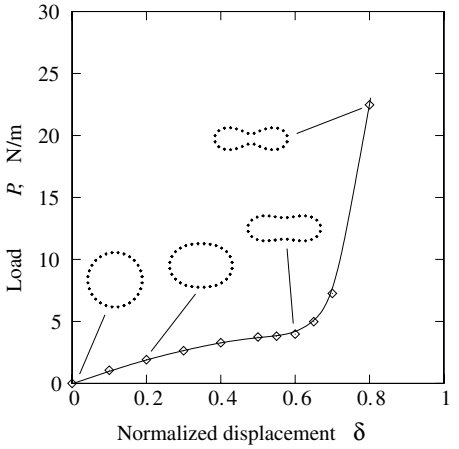

Fig. 5. Change in load of (14,0) CNT under radial compression.

rapid increase of the load over $\delta = 0.7$ is explained by the repulsion between the top and the bottom walls, because the distance between the upper and the lower wall at $\delta = 0.7$ is about 0.33 nm, which is smaller than the interlayer distance in graphite, 0.335 nm.

From the above results, we find that the deformation behavior depends on the diameter of the tubes. It should be noted that the shape of the tubes becomes back to the initial state when unloaded. This indicates that the deformation is elastic and reversible. The mechanism of the deformation behavior is summarized schematically in Fig. 6.

3.2. Change in electronic property

Fig. 7 shows the change in the band gap energy of the (8,0), (12,0) and (14,0) tubes under the radial compression. The (8,0) and (14,0) tubes have band gap energy at $\delta = 0$, which means they are semiconducting at the initial state. In both cases, the band gap decreases with the increase of the displacement and finally becomes zero, which means the transition to metallic. However, the (8,0) tube needs much smaller displacement ($\delta = 0.20$) for the transition than the (14,0) tube ($\delta = 0.55$). The result indicates that it is possible to control the sensitivity of the band gap energy to the deformation by the diameter. It is worth noting that the electric conductivity can be changed repeatedly by

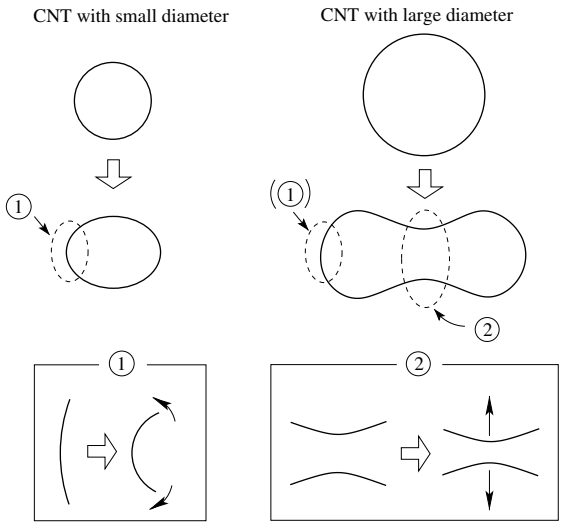

Fig. 6. Deformation mechanism of CNTs under radial compression.

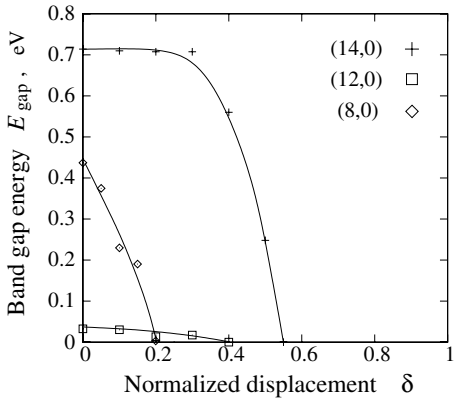

Fig. 7. Change in band gap energy under radial compression.

compression and unloading because the deformation is elastic and reversible as described in the previous section.

In the case of the (12,0) tube, which has a small band gap at $\delta = 0$, the band gap decreases gradually under radial compression. The band gap becomes null at $\delta = 0.4$, which means that this CNT also shows the transition from semiconducting to metallic.

The change in the band gap energy under the radial compression differs depending on the chiral structure, as depicted above. It has been reported that the opposite transition, from metallic to semiconducting, is observed under the radial compression in an armchair CNT [16]. As a future work, the electric property change for various chiral structures should be explored.

4. Conclusion

Tight-binding semi-empirical band calculations were performed on the radial compression of zigzag-type CNTs to investigate the mechanical and electronic properties. The results obtained are summarized as follows:

1. CNTs show large elastic deformation without bond breaking under the radial compression and the deformation is reversible.
2. The mechanical behavior during the deformation differs depending on the diameter.
3. The semiconducting CNTs show the transition to metallic under the deformation. The change in the band gap energy under the deformation depends on the chiral structure.

Acknowledgements

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