

## Damping of Unexpected Motion of Carbon-Nanotube Nanorelay-Arm by Introducing Pinhole Defects

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### Abstract

For nanorelay application of carbon nanotube (CNT), chattering motion of CNT is frequently observed. The chattering prevents reliable operations of the nanorelay. In this study, we have investigated the damping of unexpected motion of CNT arm by introducing pinhole defects on the side of CNT by using molecular dynamics simulations. The unexpected motions of CNT arm were greatly suppressed as increasing the number of the defects.

### 1. Introduction

Carbon nanotubes (CNTs) have been expected as components for high speed nanorelays because of their novel mechanical, electrical, and geometrical properties. Recently, we investigated the release of a stuck CNT cantilever beam in the nanorelay applications using not only molecular dynamic (MD) simulations [1] but also a nano-manipulator [2]. Even with strong adhesion induced by electrostatic attraction that is 100 times stronger than the van der Waals interaction, successful release of a CNT arm from a stuck state was realized by the application of a resonant vibration to the stuck CNT arm. Furthermore, nonvolatile operation of the CNT nanorelay was demonstrated by the application of the resonant vibration to the stuck CNT arm.

For the reliable switching operation of the nanorelay, the switch arm should be smoothly recovered to its original state, from on- to off-state and from off- to on-state without unexpected motion such as chattering. However, we frequently observed the unexpected motion of the arm under the nanorelay operation. In this study, we have investigated the motion of the CNT arm with pinhole defects on the side of CNT in order to suppress the unexpected motion by using the MD simulation.

### 2. Model for MD simulations

We set up the model for the nanorelay that composed with a (5, 5) single wall CNT cantilever arm with a length of ~10 nm as the active element and a graphene sheet as the counter electrode as shown in Fig. 1, where one end of the CNT was fixed and another end was free. A counter electrode of a graphene sheet was set under the free end of the CNT arm with a gap of 3.6 Å which corresponds to 0.2 Å

wider than the equilibrium position. The free end of the CNT was initially trapped by the Van der Waals (vdW) interaction with the graphene sheet. To apply the external vibration to the CNT arm, the positions of the fixed end were modulated with certain frequencies and amplitudes. In the simulation, all of atoms consisting of the graphene were fixed, so that the graphene sheet was never deformed during the simulations. To control the movement of the CNT arm, the artificial one or three pinhole defects were introduced on the side of CNT as shown in Fig. 1. We performed MD simulations with an empirical potential field of a Brenner-type potential and a Lennard-Jones type potential for an intra-CNT interaction and an inter-CNT-graphene vdW interaction, respectively. Time step for the calculation was 1 fs. To maintain the system temperature, a Berendsen bath coupling method was applied

### 3. Effect of thermal Energy

In order to clarify thermal effects without the additional external vibration, we have simulated the model at the temperature of 1500K. Figure 2 shows the temporal variation of the height of the free end of CNT arm according to the x-axis (vertical direction to the graphene plane). The CNT without defect and with one defect were released from the graphene. On the other hand, the CNT with 3 defects was not released from the graphene. It should be noted that the Young's moduli of CNTs with a few pinhole defects were not significantly degrade.[3] Thus, the stiffness degradation induced by the pinhole defects is negligible. For cantilevered CNT, we have clarified that the dissipation of

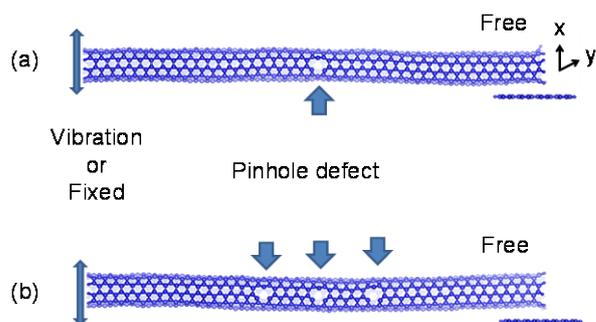


Fig. 1. Models for MD simulations. (a) CNT arm with single pinhole defect and (b) 3-pinhole defect

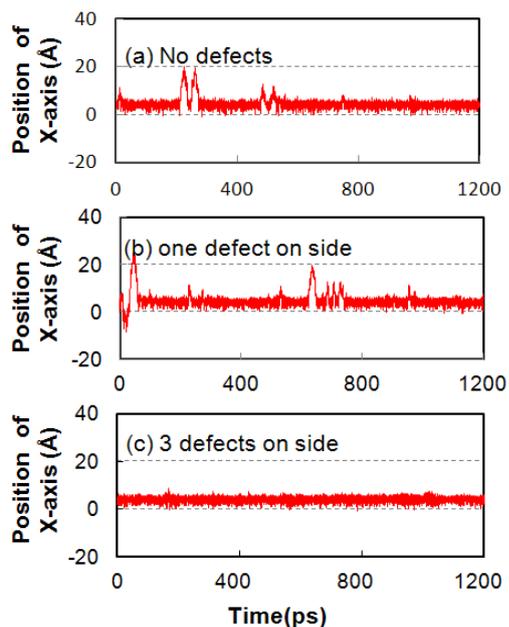


Fig. 2. Temporal variation of the tip height at 1500K: (a) No defect (b) single defect, and (c) 3-defects.

vibration energy of the cantilevered CNT is mainly induced by the introduction of the pinhole defects.[4] Consequently, the excess thermal energy mainly dissipated around the defects, so that the thermal vibration of the CNT is effectively damped.

#### 4. Release by Mechanical vibrations

We applied the external vibrations with the amplitude of  $0.9\text{\AA}$  with a frequency  $\sim 10\%$  lower than the resonant

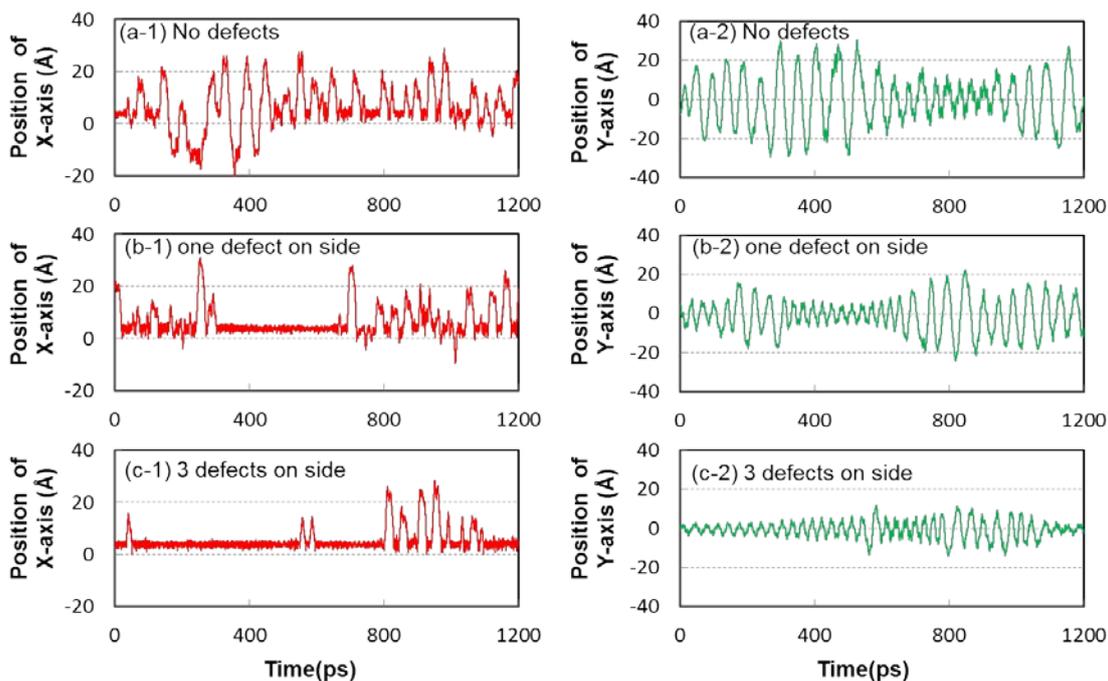


Fig. 3 Temporal variation of the tip height (red lines, x-direction indicated in Fig. 1) and the sliding amplitude on the graphene (green lines, y-direction) induced by the external vibration at 300K for no defect (a-1), (a-2), One defect (b-1), (b-2), and 3-defects (c-1), (c-2).

frequency of the stuck CNT arm. Figure 3 shows the temporal variations not only for height of (red lines) but also the sliding amplitude on the graphene sheet (green lines). As the number of the defects is increased, the unexpected release of the CNT arm due to the chattering is obviously decreased, while the stuck CNT arm can be released by application of the external vibration. Furthermore, the sliding amplitude is also effectively suppressed from 11 to  $3.5\text{\AA}$  by introduction of the pinhole defects. These damping of the unexpected motion of the CNT arm originates from the effective dissipation of the mechanical energy around the defects. Thus, we successfully control the motion of the CNT arm by introducing the defects on the side of the CNT arm.

#### 5. Conclusions

We have investigated the effects of the defects with the CNT arm on the nanorelay operation by using the MD simulations. By introducing the defects on the side of CNT arm, the unexpected motions such as chattering and sliding were successfully suppressed without the degradation of nanorelay operation.

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