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Molecular dynamics simulations for release of sticking carbon nanotube cantilever beam toward nanorelay application

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1. Introduction

Individual carbon nanotubes (CNTs) have been proposed as components for mechanical oscillators[1] and nanorelays[2] because of their novel mechanical, electrical, and geometrical properties. Such nanoscale mechanical systems are actually useful for high-sensitivity mass detection[1] and electromechanical systems[3]. For the nano-relay applications, nano-electromechanical system (NEMS) using CNTs would directly achieve smaller size, higher-frequency operation, and higher durability. The nanorelay has several advantages such as low leak current, low energy consumption, and robust to the outer perturbations.

However, there was a big demand for the reliable operation of the nanorelay. For the repeated 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. In nano-scale, sticking of the switch arm on the counter electrode takes place very frequently. While we can prevent this "sticking" by using the switch arm with high stiffness, this results in the high operation voltage and causes the serious damage to the switch contact. Recently, the reliable operation has been achieved by using a diamond thin film for the counter electrode.[2] In this case, while the electrode degradation was eliminated, the operation voltage was still higher than 20 V due to high contact resistance and high stiffness of the nanotube arm. Thus, the sticking problem should be solved to realize the reliable and low voltage operation.

In this study, we investigate the sticking nanotube arm from a counter electrode by molecular dynamics (MD) simulations and demonstrate the release of nanotube arm by adding an external mechanical perturbation.

2. Model for MD calculation

We performed MD simulations to analyze the sticking phenomena, where an empirical potential field of a Brenner-type potential and a Lennard-Jones type potential were used for an intra-nanotube interaction and an inter-nanotube-graphene vdW interaction, respectively. Time step for the calculation was 1 fs.

Figure 1(a) shows a calculation model, where a (5,5) single-wall nanotube (SWNT) cantilever beam with a length of ~ 10 nm was examined. One end of the SWNT was fixed and another end was free. A counter electrode of a graphene sheet is set under the tip of the free end of the SWNT cantilever. In this calculation, all of atoms consisting of graphene were fixed, so that the graphene sheet was never deformed during the simulations.

Initially, the free end of SWNT was trapped on the graphene sheet by the van-der-Waals (vdW) interaction at 300 K as shown in Fig. 1(b). This indicates that the sum of the strain energy induced by the bending of SWNT and the thermal energy was smaller than the vdW energy, where the vdW energy between the SWNT cantilever and the counter electrode of graphene sheet is ~ 0.8eV. This status is so-called "sticking" cantilever beam. Once the nanorelay moves to the on-state under the "sticking" condition, the nanorelay would never recover the initial state (off-state) without another perturbation at 300K.

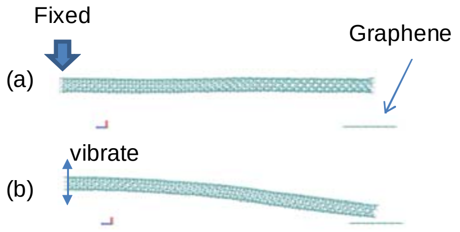

Fig. 1. Model for MD simulations: (a) before pull-in and (b) after pull-in without electrostatic attraction, namely “sticking” state.

3. Effect of thermal Energy

In order to clarify the thermal effect on the sticking, we have changed the temperature, T, of the model from 300 to 1500K. Figure 2(a) shows the temporal variation of heights at the tip and middle of the SWNT cantilever. At 300 K, the release of the SWNT cantilever from the sticking was not observed for the simulation period of 100 ps as shown in Fig. 2(a). However, the SWNT cantilever easily released within 50 ps at 1500 K as shown in Fig. 2(b). Assuming the prefactor of the attempt to escape frequency ν_0 to be 10^{12} Hz corresponding to the phonon frequency, the time constant for the release can be estimated from $\nu_0^{-1}\exp(E_a/k_BT)$ to be ~ 50 ps, where the energy barrier of the vdW energy E_a is ~ 0.8eV as mentioned in previous section and k_B the Boltzmann constant.

Under the sticking state, the cantilever CNT becomes the doubly clamped beam due to the sticking of the tip of the cantilever as shown in Fig. 1(b). As a result, the vibration with a cycle of ~12 ps corresponding to the resonant frequency of the doubly clumped beam can be observed at the middle of the SWNT cantilever. This cycle is much faster than the resonant frequency of the singly clamped beam (~80 ps) shown in Fig. 1(a). This vibration is induced by the thermal energy, k_BT. Under T = 1500 K, the amplitude of the vibration at the middle of the doubly clumped SWNT beam is larger than that at T = 300 K due to higher thermal enrgy. Thus, one of possible way to release the sticking cantilever is the application of the thermal energy, such as Joule heating. However, this is not useful for the practical application.

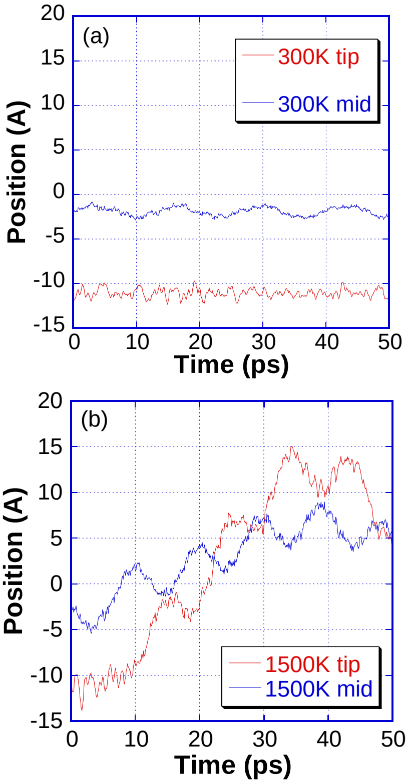

Fig. 2. Temporal variation of the tip and middle height, (a) T = 300 K, and (b) T= 1500 K.

4. Release from the sticking by mechanical vibrations

In order to stable operation of the nanorelay, the escape from the sticking is very crucial. As mentioned in previous section, the mechanical vibration can be observed even in the sticking state. If the vibration amplitude can be magnified, we expect that the kinetic energy can exceed the sticking vdW energy. Based on this concept, the vibration with the resonant frequency of the doubly clamped states with a time constant of ~ 12 ps was applied to the clamped (fixed) end of the SWNT cantilever as shown in Fig. 1(b), where the amplitude of the vibration was set to be ~ 0.09 nm at T = 300 K.

Figure 3(a) shows the temporal variation of heights at the tip and middle of the SWNT cantilever with a vibration period ~ 10 ps, which is 10% faster than that for the resonant frequency of the doubly clamped beam. In this case, while the vibration amplitude is slightly enhanced before 40 ps, the amplitude is attenuated after 40 ps. On the other hand, under the condition of the resonance of ~ 12 ps, the vibration amplitude grows with time just before the release of the sticking at ~50 ps and the sticking state is successfully released as shown in Fig. 3(b). It should be noted that the released strain energy induced the additional vibration of the SWNT cantilever with its resonant and the tip returned to the sticking position. However, this problem can be solved by using SWNTs with low Q factor. Thus, the application of the resonant vibration at the sticking state is very efficient way for the release from the sticking.

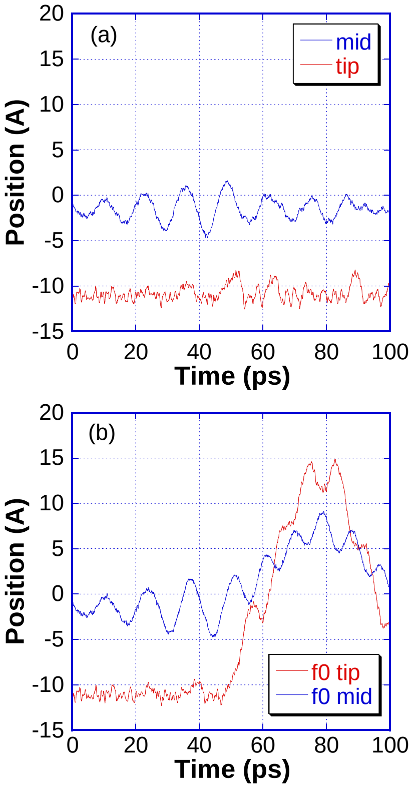

Fig. 3. Temporal variation of the SWNT cantilever at the tip and middle under the applications of vibration to the clamped end with periods of (a) ~ 11 ps (off-resonant) and (b) ~12 ps (resonant).

5. Conclusions

We have investigated the release of the sticking SWNT cantilever beam by the MD simulations. The application of the resonant vibration for the doubly clamped beam was very efficient for the release from the sticking state. We believe that this method is pave the way for practical application of the nanorelay.

References

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