Computational Study of Electron Irradiation Effects on Vibrational Properties of Carbon Nanotube Cantilevers

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Carbon nanotubes (CNT) have demonstrated exceptionally strong mechanical properties. This enables potential nanosystem functions such as large nonlinear deflections in nanotube supported structures and resonant sensors with molecular level mass sensitivity.

On another front, irradiating high energy electron to carbon nanomaterials is expected to become a technique to tailor the structure with desirable properties. However, the mechanical properties of electron-irradiated carbon nanomaterials are not well understood. We have previously reported molecular dynamics (MD) studies of electron-irradiation effects in carbon nanomaterial. [1,2] In the present work, the vibrational properties of electron-irradiated single-walled carbon nanotubes (SWCNT) are studied with the simulation.

Figure 1 shows the schematic diagram of electron irradiation region in SWCNT. The length of SWCNT is 60 Å. The carbon nanotubes with fixed ends are irradiated by electrons. The interaction between an incident electron and a carbon atom in the target nanotube is modeled based on the binary collision theory using the elastic collision cross section. Motion of each carbon atom in the nanotube under electron irradiation is calculated with the MD simulation. Three irradiated regions are selected, which label region A (10 Å to 20 Å), region B (25 Å to 35 Å) and region C (40 Å to 50 Å). The SWCNT is irradiated by 200 keV electrons at 300K.

Figure 2 shows irradiation time dependence of vibrational properties ((a) 5 ns, (b) 30 ns). In the case of irradiating at region A, the frequency decreases as the irradiation time increases. On the other hand, in the case of irradiating at region C, the frequency hardly changes even if the irradiation time increases.

From the present study, in the CNT cantilever, the frequency of the CNTs irradiated at the base get lower than that irradiated at the end. The simulations show the capability of mechanical modification of CNTs to a variety of vibrational modes by electron irradiation.

This work was supported by JSPS KAKENHI Grants number 25249052.

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[1] M. Yasuda et al., Phys. Rev. B **75**, 205406 (2007).

[2] K. Tada et al, Microelectron. Eng. 107 (2013) 50.

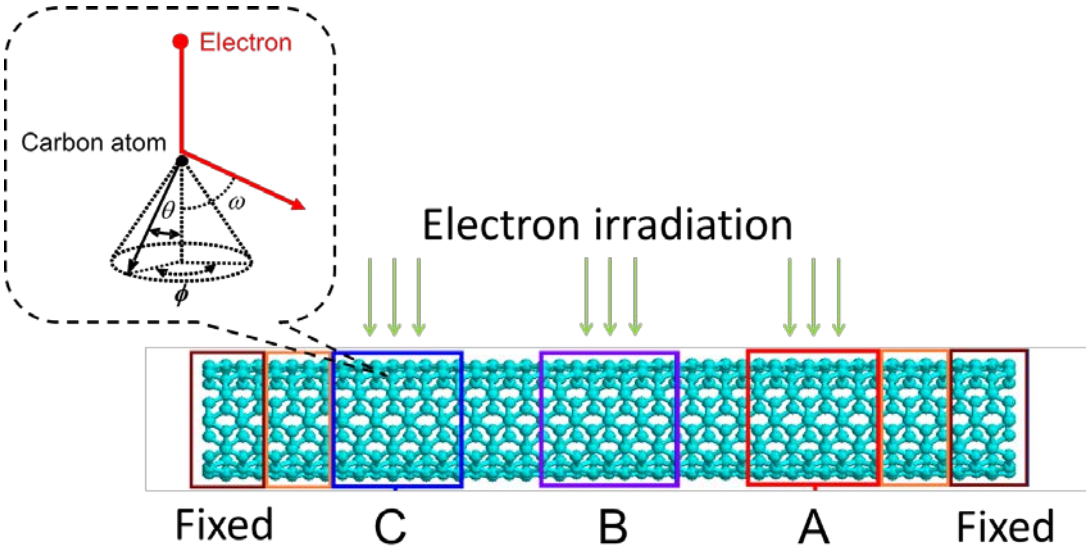
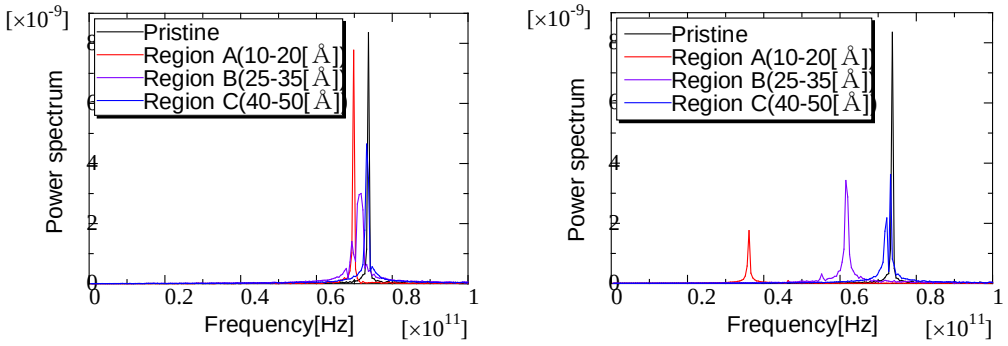


Fig. 1: Schematic diagram of electron irradiation region in SWCNT.



(a) 5 ns irradiation (b) 30 ns irradiation

Fig. 2: Irradiation time dependence of vibrational properties.