Molecular Dynamics Study on Bending Deformation of Carbon Nanotubes by Electron Beam Irradiation

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Irradiating nanomaterials with energetic particles is expected to become a technique to tailor the structure with desirable properties.[1] We have recently developed a molecular dynamics (MD) simulation including the interaction between a high energy incident electron and a target carbon atom to study structural changes of carbon nanomaterials under electron irradiation.[2] In the present work, we study the bending deformation of carbon nanotubes (CNTs) by focused electron beam irradiation with the simulation.

Figure 1 shows the configuration and the model of the simulation. The interaction between an incident electron and a carbon atom is modeled based on the binary collision theory using the Rutherford cross section. The collision atom in the CNT is randomly selected. Under the electron irradiation, the motion of each atom in the CNT is calculated with MD simulation.

Figure 2 shows the bending deformation of a (8,8) type single-walled carbon nanotube (SWNT) by 200 keV electron beam irradiation calculated by the present simulation. The temperature of both ends of the SWNT is kept constant at 1000 K. The pink circle shows the irradiated area. Only one side of the SWNT is irradiated by the electrons. The collision rate is 120 electrons/ps. The snap shots of the SWNT before and after 15 ns irradiation are shown. Several carbon atoms are ejected by the electron irradiation and the irradiated side of the SWNT shrinks through the dangling bond saturation. This results in the bending of the SWNT.

Figure 3 also shows the bending deformation of a (5,5) type SWNT. Two different sides of the SWNT are irradiated by the electrons. The beam energy, collision rate and irradiation time are 200 keV, 20 electrons/ps and 12.5 ns, respectively. The bending is seen at two positions in the SWNT after irradiation.

Our simulation results show the controllability of the bending of CNTs by selecting the conditions of electron irradiation.

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1. A. V. Krashennikov and F. Banhart, Nat. Mater. **6**, 723 (2007).
2. M. Yasuda et al., Phys. Rev. B **75**, 205406 (2007).

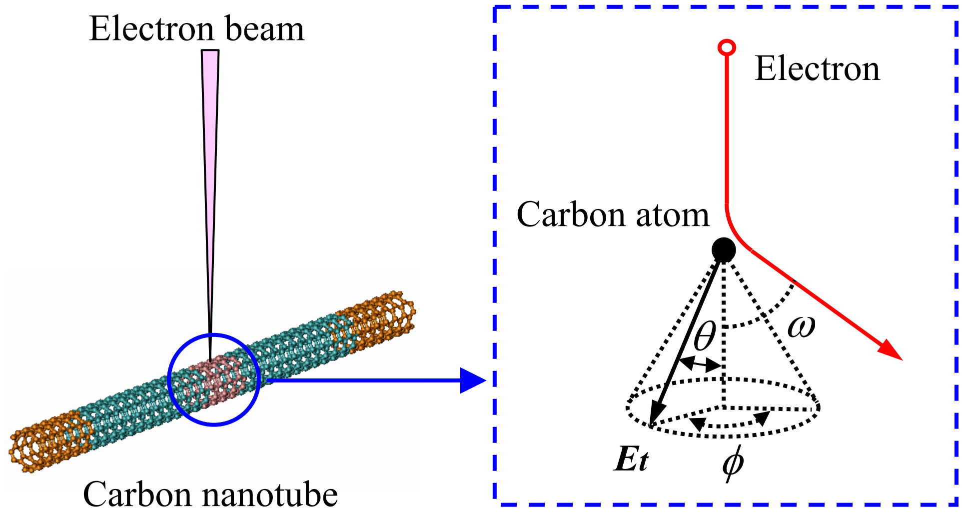

Fig. 1：Configuration and model of the simulation. The scattering angle of the incident electron ω is determined using the Rutherford cross section. The transferred energy E_t and the scattering angle of the carbon atom θ is calculated based on the binary collision theory. The scattering angle ϕ is distributed uniformly.

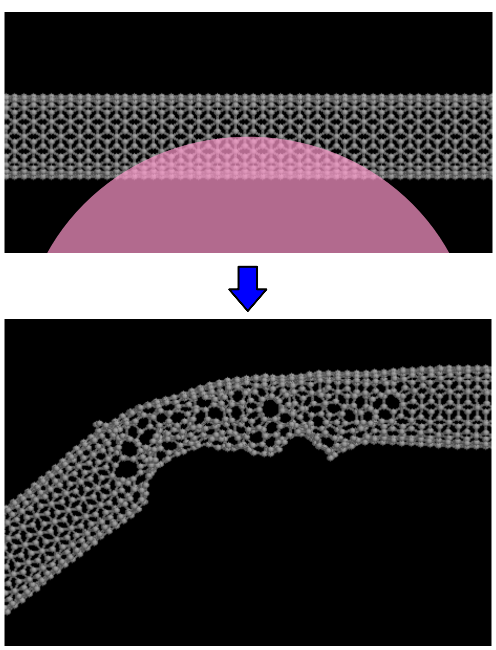

Fig. 2：The bending deformation of a (8,8) type single-walled carbon nanotube by 200 keV electron beam irradiation.

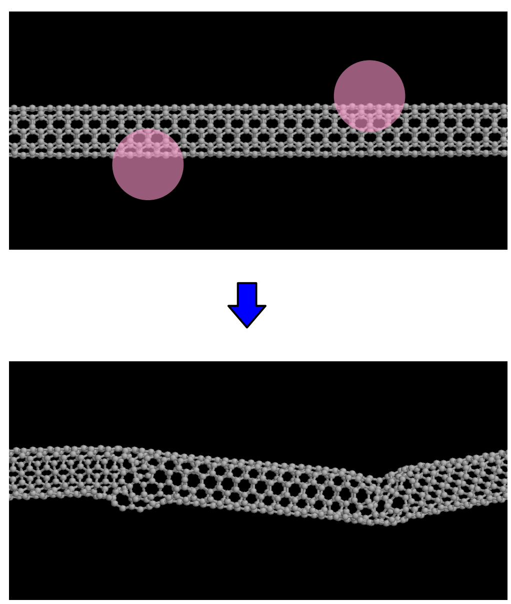

Fig. 3：The bending deformation of a (5,5) type single-walled carbon nanotube by 200 keV electron beam irradiation. Two different sides are irradiated by the electrons.