Correlation between Electron-Irradiation Effect and Stress in Carbon Nanotubes: Molecular Dynamics Study

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Structural control and modification are important to fabricate carbon nanomaterial-based nanodevices because the properties of the material strongly depend on its structure. Irradiating nanomaterials with energetic electrons is expected to become one of the techniques to tailor the structure with desirable properties. We have reported the structural changes of carbon nanomaterials under electron irradiation with a molecular dynamics (MD) simulation.[1,2] Electron energy, sample temperature and applied stress are parameters to control the structure by electron irradiation. In the present work, we study the electron-irradiation effects in carbon nanotubes under tension or torsion stress with a MD simulation.

Figure 1 shows the configuration of the present simulation. The carbon nanotubes under tension or torsion stress 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.[3] Motion of each carbon atom in the nanotube under electron irradiation is calculated with the MD simulation.

Figure 2 shows examples of the defect structures observed in carbon nanotubes after electron irradiation in the present simulation. (a) Stone-Wales and (b) adatom-vacancy defects are observed in (8,8) single-walled carbon nanotube (SWNT) as typical defects.

Figure 3 shows ratios of defect structures observed in (8,8) SWNTs after 200 keV electron irradiation for various expansion and contraction rate. The pristine tube length is 6 nm. The number of knock-on defects is not affected by both tension and compression stress so much. On the other hand, Stone-Wales and adatom-vacancy defects increase when the applied stress becomes large. From the present study, it is found that the applied stress is one of the important parameters to control the structural change in carbon nanotubes by electron irradiation.

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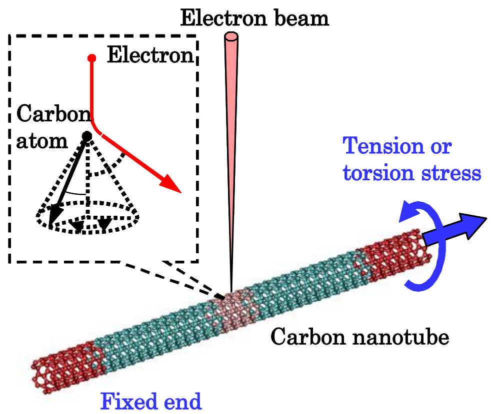

Fig. 1: Configuration of the present simulation. Carbon nanotubes under tension or torsion stress are irradiated by electrons.

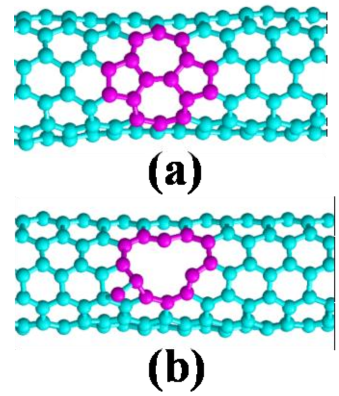

Fig. 2: Examples of the defect structure observed in (8,8) carbon nanotube after electron irradiation: (a) Stone-Wales and (b) adatom-vacancy defects.

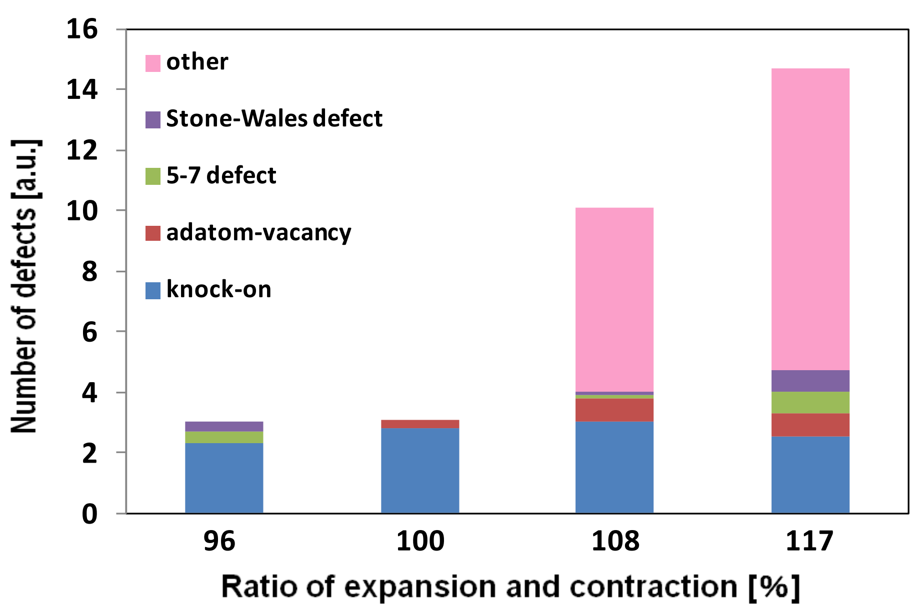

Fig. 3: Ratios of defect structures observed in (8,8) carbon nanotubes after 200 keV electron irradiation for various expansion and contraction rate.