Computational Study of Electron-Irradiation Effects in Carbon Nanomaterials on Substrates

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Irradiating nanomaterials with energetic electrons is expected to become a technique 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] In those studies, carbon materials were isolated and no supporting material was considered. For the technological application, the nanostructures supported by the substrates are also important. In the present work, we study the electron-irradiation effects in carbon nanomaterials on the substrates with a MD simulation.

Figure 1 shows the configuration of the present simulation. The interaction between an incident electron and a carbon atom in the target material is modeled based on the binary collision theory using the Mott cross section. The collision between the backscattered electron from the substrate and the carbon nanomaterial is also considered. The energy and angular distributions of backscattered electrons are calculated by a Monte Carlo simulation of the electron scattering.[2] Figure 2 shows an example of electron trajectories in Si substrate at 150 keV. The collision atom in the target material is randomly selected. Under the electron irradiation, the motion of each atom in the target material is calculated with MD simulation.[3]

Figure 3 shows the structures of double-walled carbon nanotubes (DWNT) after 150 keV electron irradiation calculated by the present simulation. The collision rate and the irradiation time are 60 electrons/ps and 500 ps, respectively. Structural changes of the isolated DWNT (Fig. 3(a)) and the DWNT on the Si substrate (Fig. 3(b)) are compared. In both structures, cross-links between the inner and outer tube-walls are observed as typical irradiation damages. The number of cross-links in the DWNT on Si substrate is larger than that in the isolated DWNT because of the collision with the backscattered electrons from the substrate.

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[1] M. Yasuda et al., J. Appl. Phys., in press.

[2] M. Yasuda et al., J. Appl. Phys. **77**, 4706 (1995).

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

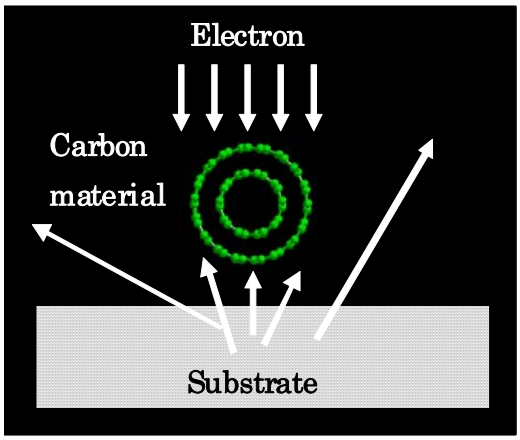

Fig. 1: Configuration of the present simulation. Carbon nanomaterials on the substrate are irradiated by the electrons.

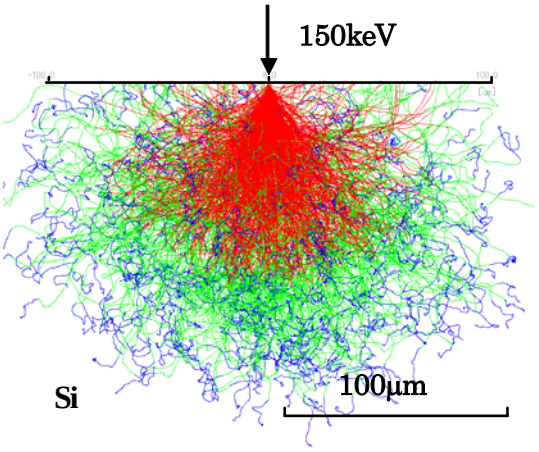

Fig. 2: Electron trajectories in Si substrate calculated by Monte Carlo simulation of electron scattering. Incident electron energy is 150 keV.

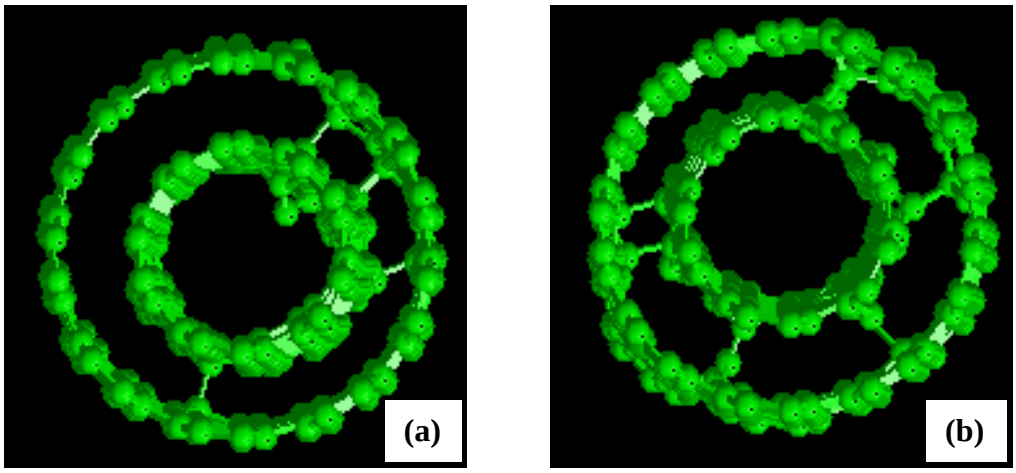

Fig. 3: Structures of the DWNTs after 150 keV electron irradiation. Structural changes of (a) the isolated DWNT and (b) the DWNT on the substrate are compared.