Molecular Dynamics Study on Structural Modifications of Graphene by Electron Beam Irradiation

Y. Asayama, Y. Chihara, M. Yasuda, H. Kawata and Y. Hirai

Department of Physics and Electronics, Osaka Prefecture University, 1-1 Gakuen-cho, Naka-ku, Sakai, Osaka 599-8531, Japan
yasuda@pe.osakafu-u.ac.jp

The control of the structural changes in nanomaterials under charged particle irradiation is one of the important issues to realize the nano-fabrication technique with charged-particle beams. We have reported the study on the structural changes in electron-irradiated carbon nanotubes with a molecular dynamics (MD) simulation.[1,2] In the present work, we report the MD study on the structural modification of graphene with electron beam.

The simulation model is the same as that we previously reported.[3] The interaction between a carbon atom and an incident electron is introduced based on the binary collision theory using the Mott cross section. The collision atom in the graphene is randomly selected. The motions of the carbon atoms under electron irradiation are calculated with the MD simulation.

As an example of the simulation results, we show here the cutting of graphene with electron beam. Figure 1 shows Snap shots of the structure of graphene during cutting process with 200 keV electron beam obtained by the present simulation. The electron collision rate is 10 electrons/ps. The irradiated area is shown by the colored rectangle in Fig.1(a). The width of the irradiated area is 1.0 nm. After the irradiation for 55 ns, the graphene is perfectly divided into two pieces as shown in Fig.1(c). However, the shapes of the cutting edges are disorderly. Atomic chains are frequently observed at the cutting edges.

Figure 2 shows the number of knock-on carbon atoms from electron-irradiated graphene as a function of irradiation time. The electron energy is 200 keV. The numbers of knock-on atoms increases linearly with the irradiation time for both the electron collision rates of 5 and 10 electrons/ps.

Figure 3 shows the number of knock-on atoms from electron-irradiated graphene as a function of electron energy. Although the statistical fluctuation is observed in the result, the knock-on atoms increase with the increase in the electron energy. The knock-on of the carbon atom occurs above 110 keV in the simulation.

This work was supported by the Grants-in-Aid for Scientific Research from the Japan Society for the Promotion of Science.

---

[1]M. Yasuda et al., J. Appl. Phys. **109**, 054304 (2011).

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

[3]Y. Chihara et al., J. Vac. Sci. Technol. B **29**, 06FG09-5 (2011).

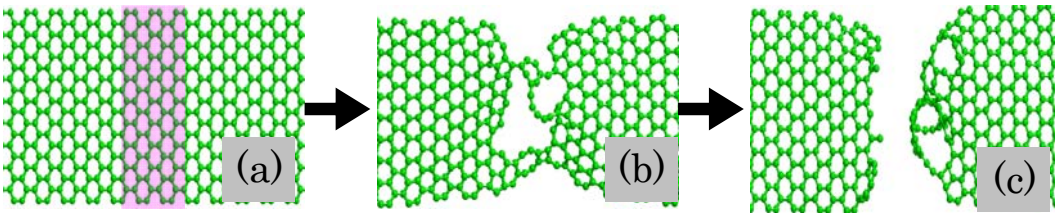

Fig. 1: Snap shots of the structure of graphene during cutting process with 200 keV electron beam. Irradiation times are (a) 0 ns, (b) 30 ns and (c) 55 ns.

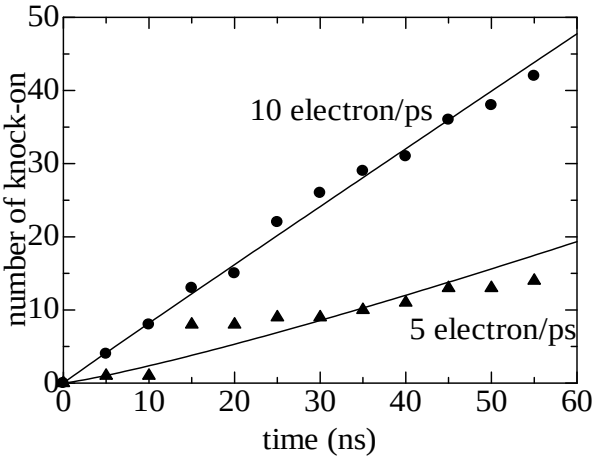

Fig. 2: The number of knock-on atoms from electron-irradiated graphene as a function of irradiation time. The electron energy is 200 keV. The collision rates are 5 and 10 electrons/ps.

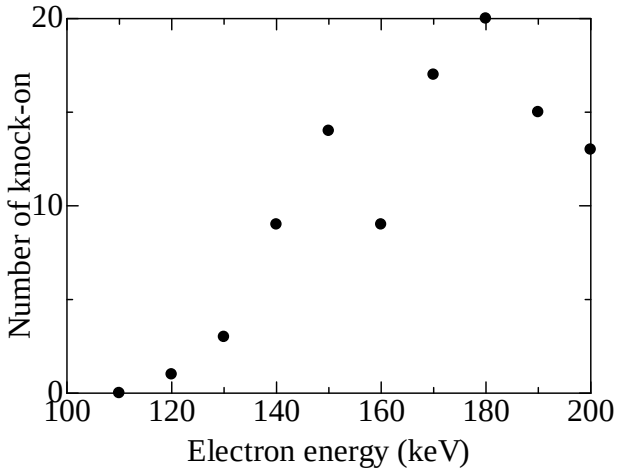

Fig. 3: The number of knock-on atoms from electron-irradiated graphene as a function of electron energy.