Structural Change of Graphene during Electron Beam Process: Molecular Dynamics Study

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The electron beam process is one of the important technologies to tailor the carbon nanostructure with desirable properties. Understanding of the atomic level behaviors of the materials under electron irradiation is indispensable to realize the precise structure control.[1] In the present work, we report the molecular dynamics (MD) study on the structural change of graphene under electron irradiation.

The simulation model is the same as that we previously reported.[2] 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.

Electron irradiation causes several types of structural changes such as knock-on, pentagon-heptagon (5-7) and Stone-Wales defect. Figure 1 shows the variation of the potential energy of graphene before and after 5-7 defect formation by electron collision. When the electron collision provides larger energy than the activation energy, 5-7 defect is formed in honeycomb network of graphene. The potential energy of the structure rises about 5 eV after 5-7 defect creation.

Figure 2 shows the process of the structural change of the graphene nanoribbon under 200keV electron irradiation at 1500 K. Along with ejection of carbon atoms by the electron collision, the high temperature also promotes reconstruction of the carbon network. The structure becomes amorphous-like graphene. In this process, the structure is composed of mostly 5-7 defects and reconstruction to the hexagon rich structure occurs. With the increase of knock-on defects, the amorphous-like graphene becomes narrower. The structure becomes a single atomic chain finally.

Figure 3 shows (a) the number of six-membered rings and (b) potential energy of electron-irradiated graphene nanoribbon with irradiation time. The data at A - F correspond to the structures in Fig. 2. Under the irradiation, the number of six-membered rings does not simply decrease but fluctuates due to the competition between the defect formation by electron collision and the recovery by annealing. In the recovery process, the potential energy decreases as shown in Fig. 3 (b).

This work was supported by JSPS KAKENHI Grant Number 25249052.

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

[2] Y. Asayama et al., J. Vac. Sci. Technol. B **30**, 06FJ02 (2012).

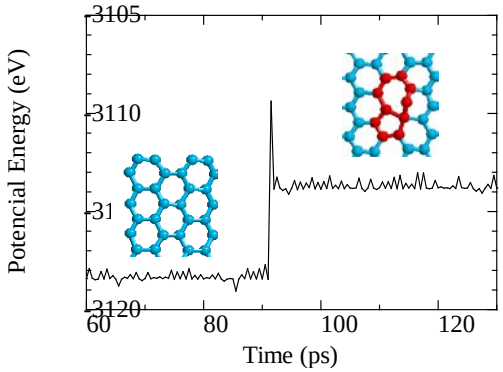

Fig. 1: The variation of the potential energy of graphene before and after the 5-7 defect formation by electron collision.

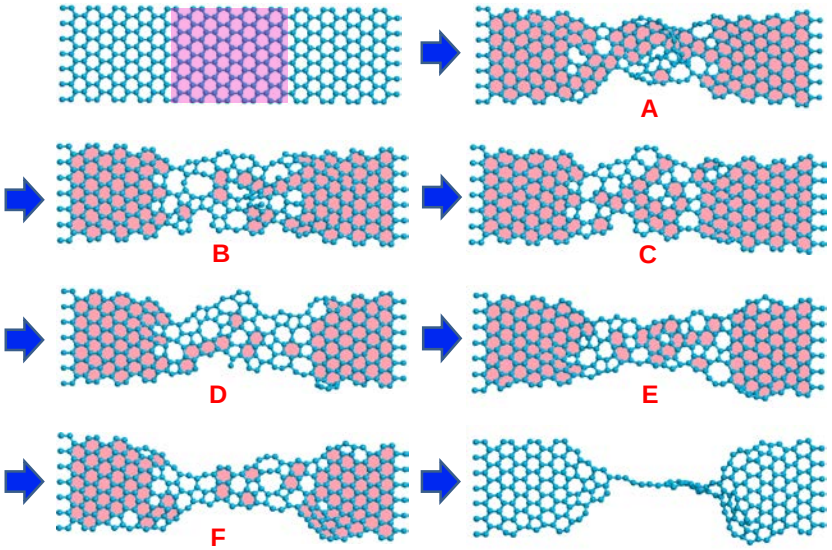

Fig. 2: Structural change of graphene nanoribbon under 200keV electron irradiation.

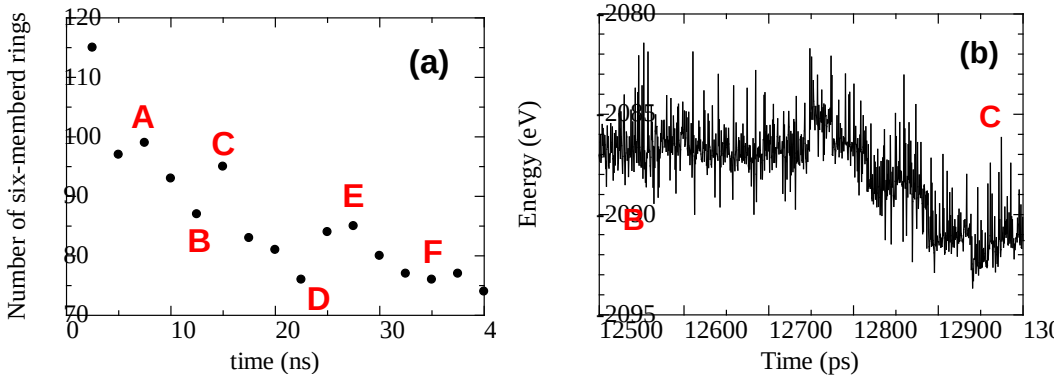

Fig. 3: (a) The number of six-membered rings and (b) the potential energy of electron-irradiated graphene nanoribbon as a function of electron irradiation time.