Molecular dynamics study of thermal properties of graphene during electron irradiation

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The nanostructures are frequently observed by the electron microscope and the properties of nanomaterials are also measured under electron microscope observation. The temperature rise of the materials caused by electron irradiation affects those observed structures and measured properties. Therefore, the temperature of the materials under electron irradiation is one of the important factors for electron microscope observation. Furthermore, the thermal managements of materials and devices become growing concern in the recent technology. The electron-beam testing can become a potential candidate as evaluation method of thermal properties of nanomaterials. However, information about the temperature of the nanomaterials during electron microscope observation is few. In the present work, the heating and thermal transport properties in the electron-irradiated graphene are studied by the molecular dynamics (MD) simulations. The effects of electron irradiation conditions and graphene structures on thermal properties are investigated with the simulation.

The motions of carbon atoms in graphene are calculated using the MD simulation with empirical potentials. The electron irradiation effects are periodically introduced into the MD simulation by the same model we previously reported [1, 2]. The collision atoms are randomly selected. The scattering angle of an incident electron is determined using the elastic collision cross section. Then, the momentum transfer from an electron to a carbon atom is calculated by the binary collision theory. The temperature distribution of graphene is estimated from the kinetic energies of constituent carbon atoms.

Figure 1 shows an example of the configuration of the present simulation. The temperature distribution of the square-shaped graphene under focused electron beam irradiation is calculated. All four edges of graphene are fixed. The temperature of those fixed edges is kept constant at 300 K and the edges act as heat sinks. The center region of the graphene is irradiated by the electrons. Figure 2 shows the temperatures of the electron-irradiated region of graphene as a function of irradiation time. The temperatures rise with increasing irradiation time. Although the temperature fluctuates due to the statistical effect of electron collision, the temperature increases with decreasing acceleration voltages. Figure 3 shows another example of the configuration of the simulation. The thermal transport property of defective graphene nanoribbon under electron irradiation is calculated. The narrow edges of nanoribbon are fixed. The temperature of those fixed edges is kept constant at 300 K. The left side of the nanoribbon is irradiated by the electrons. The temperature is monitored in the region surrounded by the rectangular. Several mono-vacancy defects are introduced in nanoribbon between the irradiated and measuring regions. Figure 4 shows the temperatures of the graphene nanoribbons as a function of electron irradiation time. The acceleration voltage is 100 kV. The temperature rises slower when the number of mono-vacancy defects increases. In conclusion, while the heat generation is mainly determined by the electron irradiation conditions, the heat transportation is affected by graphene structures.

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

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

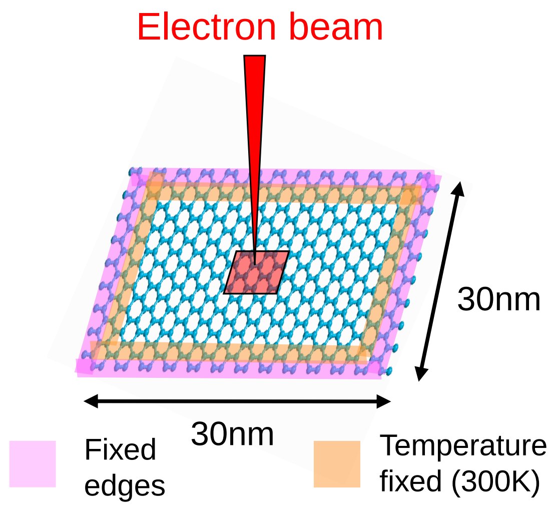

Fig. 1 Configuration of heating simulation in electron irradiated square-shaped graphene.

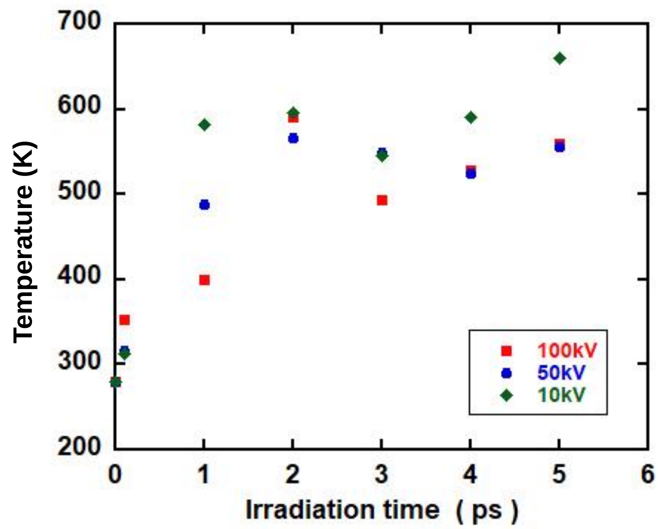

Fig. 2 Temperature of square-shaped graphene as a function of electron irradiation time.

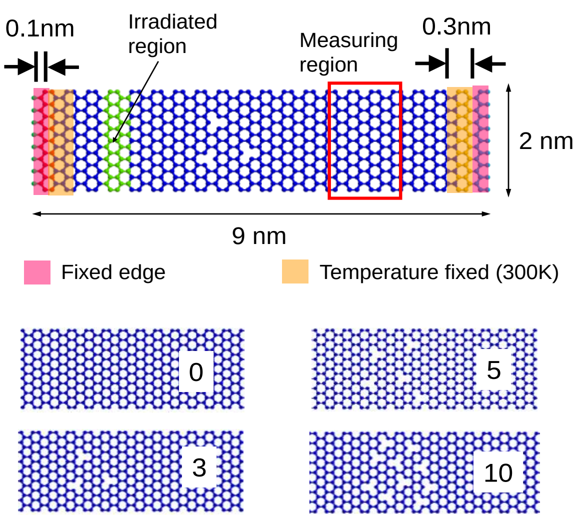

Fig. 3 Configuration of thermal transport simulation in electron irradiated graphene with mono-vacancy defects.

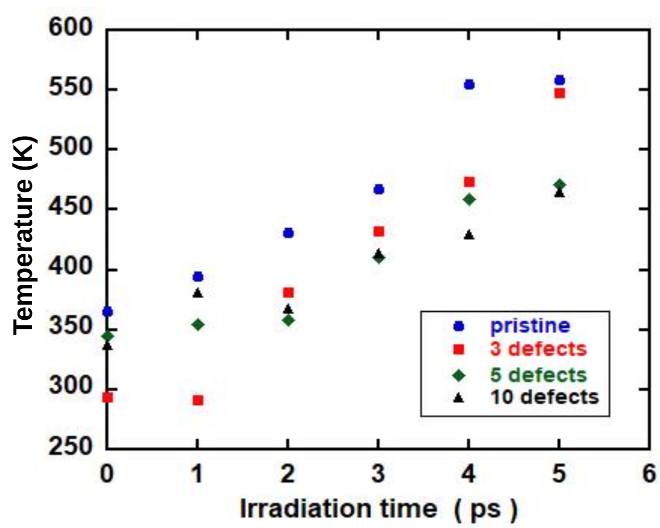

Fig. 4 Temperature of defective graphene nanoribbon as a function of electron irradiation time.