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The vacancy diffusion and the formation of dislocation in graphene : Tight-binding molecular dynamics simulation

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Vacancy defects in graphene can be created by electron or ion irradiation and those induce ripples which can change the electronic properties of graphene. Recently, the formation of defect structures such as vacancy defects and non-hexagonal rings has been reported in the high resolution transmission electron microscope (HR-TEM) of reduced graphene oxide [1]. In those HR-TEM images, it is noticed that the dislocations with pentagon-heptagon (5-7) pairs are formed and diffuses. Interestingly, it is also observed that two 5-7 pairs are separated and diffuse far away from each other. The separation of 5-7 pairs has been known to be due to their self-diffusion. However, from our tight-binding molecular dynamics simulation, it is found that the separation of 5-7 pairs is due

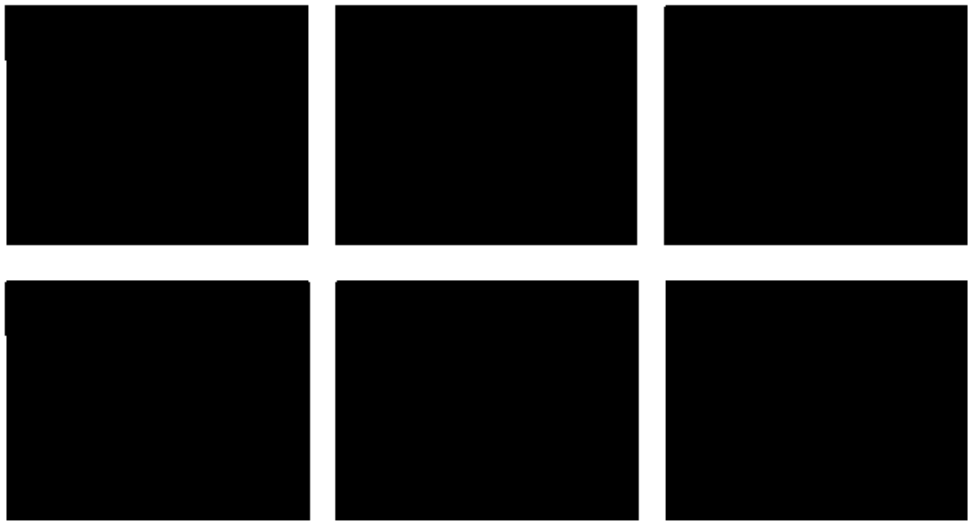

Figure : The separation of 5-7 pairs by the diffusion and coalescene of single vacancy defects

to the diffusion of single vacancy defects and coalescence with 5-7 pairs. The diffusion and coalescence of single vacancy defects is too fast to be observed even in HR-TEM. We also implemented Van der Waals interaction in our tight-binding carbon model to describe correctly bi-layer and multi-layer graphene. The compressibility of graphite along c-axis in our tight-binding calculation is found to be in excellent agreement with experiment. We also discuss the difference between single layer and bi-layer graphene about vacancy diffusion and reconstruction.

[1] C. Gomez-Navarro et al. Nano Letters 10, 1144 (2010)