NF-006

Structural properties of vacancy defects, dislocations, and edges in graphene

Gun-Do Lee[1], Euijoon Yoon[1], Nong-Moon Hwang[1], Youngkuk Kim[2], Jisoon Ihm[2], Cai-Zhuang Wang[3], Kai-Ming Ho[3]

[1]Department of Materials Science and Engineering, Seoul National University, [2]Department of Physics, Seoul National University, [3]Department of Physics, Iowa State Univeristy

Recently, we performed ab initio total energy calculation and tight-binding molecular dynamics (TBMD) simulation to study structures and the reconstruction of native defects in graphene. In the previous study, we predicted by TBMD simulation that a double vacancy in graphene is reconstructed into a 555-777 composed of triple pentagons and triple heptagons [1]. The structural change from pentagon-octagon-pentagon (5-8-5) to 555-777 has been confirmed by recent experiments [2,3] and the detail of the reconstruction process is carefully studied by ab initio calculation. Pentagon-heptagon (5-7) pairs are also found to play an important role in the reconstruction of vacancy in graphene and single wall carbon nanotube [4]. In the TBMD simulation of graphene nanoribbon (GNR), we found the evaporation of carbon atoms from both the zigzag and armchair edges is preceded by the formation of heptagon rings, which serve as a gateway for carbon atoms to escape. In the simulation for a GNR armchair-zigzag-armchair junction, carbon atoms are evaporated row-by-row from the outermost row of the zigzag edge [5], which is in excellent agreement with recent experiments [2, 6]. We also present the recent results on the formation and development of dislocation in graphene. It is found that the coalescence of 5-7 pairs with vacancy defects develops dislocation in graphene and induces the separation of two 5-7 pairs. Our TBMD simulations also show that adatoms are ejected and evaporated from graphene surface due to large strain around 5-7 pairs. It is observed that an adatom wanders on the graphene surface and helps non-hexagonal rings change into stable hexagonal rings before its evaporation.

[1] G. -D. Lee Phys. Rev. Lett. 95, 205501 (2005)
[2] C. O. Girit et al. Science 323, 1705 (2009)
[3] J. C. Meyer (in private communication)
[4] G. -D. Lee Appl. Phys. Lett. 97, 093106 (2010)
[5] G. -D. Lee Phys. Rev. B 81, 195419 (2010)

[6] X. Jia et al. Science 323, 1701 (2009) ; A. Chuvilin et al. New. J. Phys. 11, 083019 (2009) ; C. Jin et al. Phys. Rev. Lett. 102, 205501 (2009)

Keywords: graphene, vacancy defects, reconstruction, dislocation, graphene nanoribbon, ab initio calculation, tight-binding molecular dynamics simulation