# Tight-binding Molecular Dynamics Simulation Study on Defect Structures in Graphene: Analysis of TEM images

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**Abstract**

Transmission electron microscopy technique has been developed to study the structure of materials. Two dimensional materials, such as graphene, have been an effective subject to test the TEM technique. However, it sometimes faces the limitation in the detection of short-time dynamical processes such as defect creation and reconstruction. Simulation methods are useful to elucidate detailed atomic processes which could hard to be observed in experiments even with the state-of-the-art microscope techniques. While *ab initio* simulation method are quite accurate, it focused only on total energy and band structure calculations due to the high cost in performing molecular dynamics simulation. Classical molecular dynamics simulations are sometimes questionable in their accuracy because such simulations do not contain quantum mechanical interactions. In order to overcome the limitations in the above two types of simulation methods, tight-binding molecular dynamics (TBMD) simulation method is very useful in the respect of accuracy and computational cost. The environment dependent tight-binding carbon potential is employed and it gives accurate results as those obtained by *ab initio* calculation for various defects structures. The TBMD simulations reveal interesting mechanisms for the formation and reconstruction of vacancy [1, 2], dislocation [3 - 5], and grain-boundary in graphene, which are also confirmed by *ab initio* total energy calculations. In this talk, I also discuss how we can analyze the TEM images of graphene defect structures and find the unseen processes by the aid of TBMD simulation method.

## References

[1] G.-D. Lee, C. Z. Wang, E. Yoon, N.-M. Hwang, D.-Y. Kim, K. M. Ho, *Phys Rev Lett* 95, 205501 (2005)
[2] Y. Kim, J. Ihm, E. Yoon, and G.-D. Lee Phys. Rev. B **84**, 075445 (2011).
[3] B. W. Jeong, J. Ihm, and G.-D. Lee, Phys. Rev. B **78**, 165403 (2008).
[4] G.-D. Lee, E. Yoon, N.-M. Hwang, C. Z. Wang, K. M. Ho, *Appl. Phys. Lett.* 102, 021603 (2013)
[5] J. H. Warner, E. R. Margine, M. Mukai, A. W. Robertson, F. Giustino, and A. I. Kirkland, Science 2012, 337, 209

## Figures

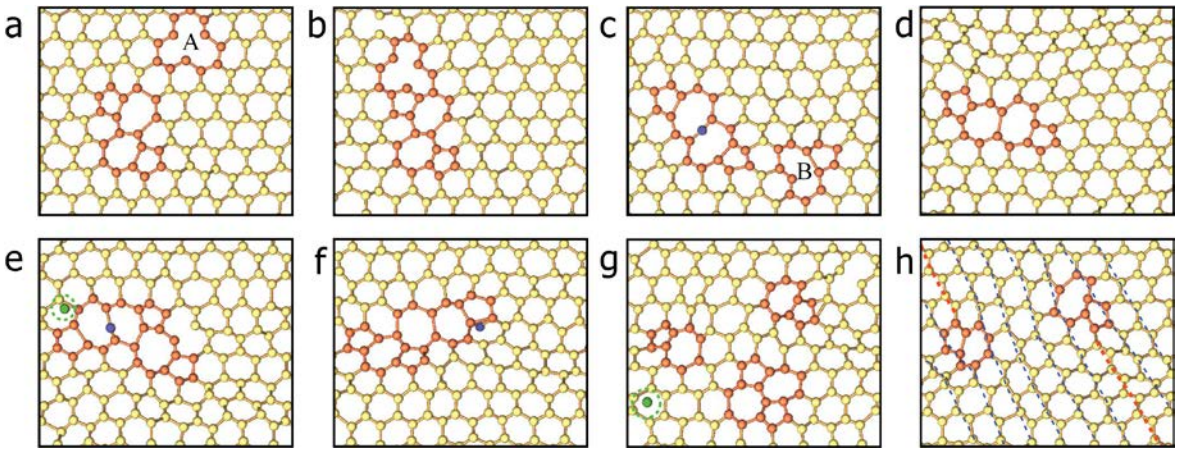


*Figure1: Snapshots from the TBMD simulation for development into dislocation from vacancy defects*

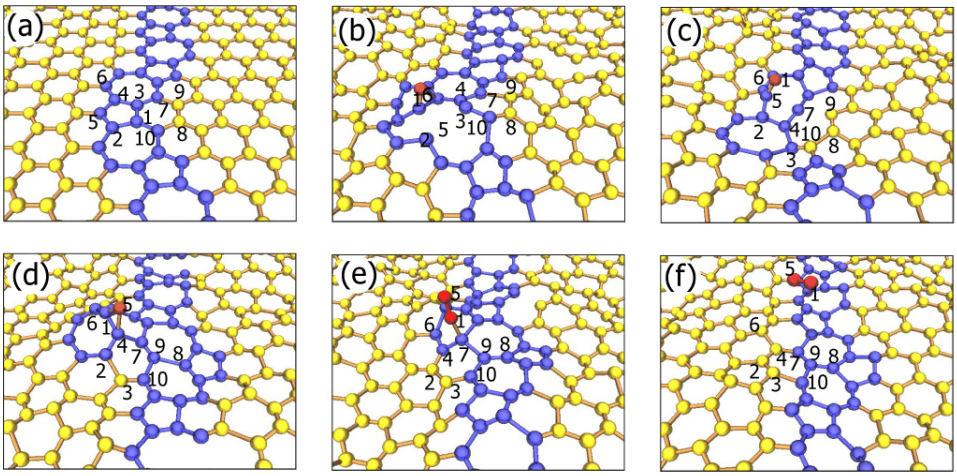


*Figure2: Snapshots from TBMD simulations for dimer evaporation from graphene grain boundary. Numbers show the trajectory of identical atoms.*