# Understanding initial dissociation process of carbon source molecules during nanotubes and graphene synthesis: *Ab initio* molecular dynamics simulations

Yasushi Shibuta[1*], Kohei Shimamura[2], Tomoya Oguri[1], Rizal Arifin[2],

Wataru Hashizume[2], Fuyuki Shimojo[2], and Shu Yamaguchi[1]

*1 Department of Material Engineering, The University of Tokyo, JAPAN*
*(*shibuta@materialt.u-tokyo.ac.jp)*
*2 Department of Physics, Kumamoto University, JAPAN*

We have investigated the initial dissociation process of carbon source molecules during the carbon nanotubes (CNTs) and graphene growth via a chemical vapor deposition (CVD) process by *ab initio* molecular dynamics (MD) simulation. In particular, we have examined the following three cases: (1) Methane dissociation on Ni(111) surface [1]. (2) Ethylene dissociation on Ni32 cluster [2] and (3) Ethanol dissociation on Ni32 cluster [3].

For example, methane molecules are dissociated into isolated carbon and hydrogen atoms via $CH_3$ and CH fragments with chemisorbing the nickel (111) surface [1]. Dissociated carbon atoms are then buried into the subsurface space between first and second nickel layers via diffusion through hollow sites in the nickel layers.

In the presentation, our recent results will be introduced and then the role of the catalytic metals on the CNTs and graphene growth at the initial stage will be discussed.

[1] Y. Shibuta, et al. Chem. Phys. Lett., 565 (2013) 92-97.
[2] K. Shimamura, et al., submitted.
[3] T. Oguri, et al., to be submitted.