Ab initio molecular dynamics study on the role of nickel cluster as catalytic metal in carbon nanotubes synthesis

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The knowledge on the formation mechanism of carbon nanotubes and the role of catalytic metals in the growth of single-walled carbon nanotubes (SWNTs) via a catalytic chemical vapor deposition method has been established over two decades [1,2]. However, the difficulty of direct experimental observation of the dissociation of carbon source molecules has caused unclear understanding of the initial stage of SWNTs formation. In present study, dissociation of ethanol molecules on the nickel cluster has been investigated by *ab initio* molecular dynamics and nudged-elastic-band (NEB) simulations to discuss the initial stage of metal-catalyzed growth process of carbon nanotubes and the role of nickel cluster as catalytic metal through an alcohol catalytic chemical vapor deposition [2]. It has been observed that both C-C and C-O bonds in ethanol molecules are dissociated on the nickel cluster. Subsequently, formations of various reaction products such as hydrogen atoms and molecules, carbon monoxide, oxygen atom, water, ethylene, methane and their fragments have occurred. In addition, the role of nickel cluster as catalytic metal is evident indicated by a decrease of the activation energy of the C-H bond dissociation in the fragment molecules, which is estimated by the NEB analysis to be approximately one-eighth of the bond-dissociation energy of the corresponding C-H bond without the influence of the nickel cluster. In the presentation, the detail catalytic role of nickel cluster will be introduced after the brief review of recent computational works on this topic.

[1] Y. Shibuta, Diamond and related Materials, 20 (2011) 334-338
[2] K. Shimamura, T. Oguri, Y. Shibuta, S. Ohmura, F. Shimojo, S. Yamaguchi, submitted.
[3] T. Oguri, K. Shimamura, Y. Shibuta, F. Shimojo, S. Yamaguchi, to be submitted.