Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ethanol decomposition on transition metal nanoparticles during carbon nanotube growth: ab initio molecular dynamics study[1] YASUSHI SHIBUTA, The University of Tokyo, KOHEI SHIMAMURA, Kumamoto University, TOMOYA OGURI, The University of Tokyo, RIZAL ARIFIN, FUYUKI SHIMOJO, Kumamoto University, SHU YAMAGUCHI, The University of Tokyo — The growth mechanism of carbon nanotubes (CNT) has been widely discussed both from experimental and computational studies. Regarding the computational studies, most of the studies focuses on the aggregation of isolate carbon atoms on the catalytic metal nanoparticle, whereas the initial dissociation of carbon source molecules should affect the yield and quality of the products [1]. On the other hand, we have studied the dissociation process of carbon source molecules on the metal surface by the ab initio molecular dynamics simulation [2,3]. In the study, we investigate the ethanol dissociation on Pt and Ni clusters by ab initio MD simulations to discuss the initial stage of CNT growth by alcohol CVD technique. [1] Y. Shibuta, Diamond and Related Materials, 20 (2011) 334-338. [2] T. Oguri, K. Shimamura, Y. Shibuta, F. Shimojo, S. Yamaguchi, J. Phys. Chem. C 117 (2013) 9983. [3] T. Oguri, K. Shimamura, Y. Shibuta, F. Shimojo, S. Yamaguchi, Chem. Phys. Lett., 595-596 (2014) 185.

[1]Part of this research is supported by the Grant-in-Aid for Young Scientists (a) (No. 24686026) from MEXT, Japan.

Yasushi Shibuta
The University of Tokyo

Date submitted: 13 Nov 2014 Electronic form version 1.4