Discussion on carbon precursor dissociation at initial stage of carbon nanotube growth

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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]. Under such circumstances, 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. In the presentation, our recent studies will be introduced after a brief review of this issue.

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[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.