Octopus and VLS mode growth of single-walled carbon nanotubes by molecular dynamics method

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In order to explore the possible chirality-controlled growth process, the growth mechanism of single-walled carbon nanotubes (SWNTs) was studied by molecular dynamics simulations. We have adopted a newly developed Tersoff-type classical potential for carbon and several metal atoms, such as Co, Ni, Pt, Fe and Ti [1]. A genetic algorithm was employed to optimize the potential functions for various solid structures and metal-on-graphene model calculated by DFT. The nucleation and growth of an SWNT from a metal cluster of certain size and at certain temperature and pressure range are observed. Here, we observe two apparently different growth modes of SWNTs. A preferred structure at lower temperature is 'Octopus' mode where several carbon chains are wrapping the metal cluster. The preference of carbon chain structure on metal surface prohibited the transition to hexagonal structure which can lead to the full encapsulation of metal cluster. Because of this chain structure, the solid-state metal cluster can be a stable catalyst. Another structure appeared at higher temperature is 'VLS' mode where carbon atoms are dissolved in liquid metal cluster. The nucleation and growth of SWNTs is dynamics process depending on carbon feeding rate. The diameter of nanotube is similar to the metal cluster size for Octopus mode in contract to the VLS mode where the diameter is determined in the dynamically nucleated cap structure. These 2 modes may correspond to 'tangential' and 'perpendicular' modes observed in TEM [2]. These 2 different growth modes may explain the drastic diameter change observed in vertical aligned CVD growth by adding nitrogen in carbon precursors [3]. Here, we found that reversible and repeatable growth of 1 nm or 2 nm diameter SWNTs from the same catalysts [3].

[1] T. Matsuo, master thesis, http://www.photon.t.u-tokyo.ac.jp/thesis/2011/2011matsuo.pdf
[2] M.-F. C. Fiawoo, *et al.*, Phys. Rev. Lett., 108 (2012) 195503
[3] T. Thurakitseree, *et al.*, ACS Nano, 7 (2013) 2205

Properties of carbon nanotube/SiC heterojunctions formed by surface decomposition of SiC

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Carbon nanotubes (CNTs)/semiconductor heterojunctions have been an important subject in nanoelectronics. However, it has been difficult to fabricate CNT/semiconductor heteojunctions, where CNTs and semiconductor surface were directly bonded at the interface, such as conventional semeiconductors. Recently, we have been investigating CNT growth by surface decomposition of SiC [1]. By this method, aligned zigzag-type CNTs with fairly uniform tube diameters can be selectively produced normal to the SiC surface. In addition, carbon atoms of the CNTs are directly bonded to SiC at the interface without any interlayers,indicating the formation of CNT/semiconductor heterojunction at the interface. In this study, we formed CNT/SiC heterojunctions and investigated the crystalline and electronic properties of the interface between CNTs and SiC using TEM and photoemission (PES).

CNT/n-type SiC heterojunctions were formed by surface decomposition of 4H-SiC(000-1). Through heating temperature and heating time, the CNT length could be controlled up to 4 μm. For the sample with CNTs of 180 and 230 nm in thickness, distinct rectifying behavior was observed in the current-voltage measurements. When the CNT length was 1500 nm, the leakage current was increased. From TEM observations, we concluded that the increase of the leakage current was due to the deterioration of crystalline quality of CNTs near the interface. We also carried out PES measurements for CNT/n-type SiC and the band bending at the interface will be discussed.

[1] T. Maruyama *et al.,* Appl. Phys. Lett. 101 (2012) 092106