CVD Growth of SWNTs and MD Modeling

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Developments of catalytic CVD generation of single-walled carbon nanotubes (SWNTs) are reviewed with an emphasis on vertically aligned (VA) growth. Following the first realization of VA-SWNTs [1] by alcohol catalytic CVD (ACCVD) method, various techniques are reported for the vertical aligned growth such as control of water [2], point-arc microwave plasma CVD [3], molecular-beam CVD [4], hot-filament control of atomic hydrogen [5], hydrogen/oxygen ratio control by oxygen-assisted CVD [6]. Later, it turns out that the optimization of catalysts and CVD conditions is enough for VA-SWNTs [7-9]. The growth condition and mechanism of VA-SWNTs is further discussed based on the in-situ growth monitoring by laser absorption [7] and the direct TEM observation of inner structure of VA-SWNT film [10].

In parallel to experimental studies molecular dynamics (MD) modeling studies are reviewed. Growth of nanotube cap structure was demonstrated by MD simulations [11]. Later, MD simulations at realistic temperatures [12] and even with *ab initio* MD [13] are discussed. Here, the structure of carbon-metal binary cluster and the carbon flow path is discussed in detail from the MD simulation results [11].

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