Controlling growth modes of SWNTs

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A detailed understanding of the catalyst/nanotube interface, under actual growth conditions, is probably a key to a selective synthesis of single wall carbon nanotube (SWNT). Through careful Transmission Electron Microscopy observations [1], so called tangential and perpendicular growth modes were identified and Grand Canonical Monte Carlo simulations based on a tight binding model for nickel and carbon alloys [2, 3, 4], were used to analyze these growth modes at the atomic scale.

Further numerical investigations presented here show that, when catalyst nanoparticles are small enough to be (partially) molten under the synthesis conditions,- i. e. with a diameter below 3 nm -, these growth modes are directly related to the average carbon content in the catalyst nanoparticles. They also show that carbon incorporation energetics and statistics at the SWNT/nanoparticle interface depend on both nanotube helicity and carbon content, thus possibly indicating a route towards a full control of the nanotube structure during synthesis

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