

Growth Modes and Chiral Selectivity of SWNTs

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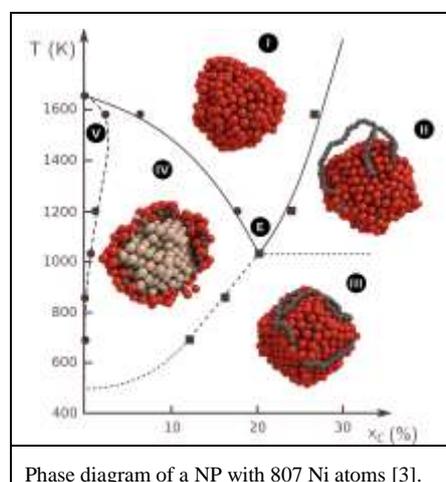
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A detailed understanding of the catalyst/nanotube interface, *under actual growth conditions*, is probably a key for a selective synthesis of single wall carbon nanotube (SWNT) by catalytic chemical vapor deposition (CCVD). I will show here how dedicated computer simulations, mostly based on a tight binding model for carbon and nickel [1], a typical catalyst, can provide a useful insight.

It starts with the complex stability pattern of atomic carbon dissolved in subsurface layers of crystalline Ni, that depends on the presence of a graphene layer on top of it [2]. For catalyst nanoparticles below 3 nm, relevant for the CCVD growth, the presence of carbon dissolved in the surface layers induces a gradual melting at temperatures well below the melting temperature of pure nanoparticles of the same size. Calculated size dependent phase diagrams for Ni-C nanoparticles [3] indicate that faceted crystalline nanoparticles are unlikely to be observed in this size range under growth conditions.

This raises the question of the role of the carbon dissolved in the catalyst during the growth, that is shown to have a strong influence on the wetting properties of the metal-SWNT interface [4]. Through careful Transmission Electron Microscopy observations [5], so called tangential and perpendicular growth modes were identified. Computer simulations were used to analyze these growth modes at the atomic scale, demonstrating that the tangential mode corresponds to a weak carbon supply and slow growth, while the perpendicular one is observed when the carbon fraction in the nanoparticle is larger [6]. Growth experiments designed to tune the carbon fraction in the nanoparticle by changing the carbon feedstock (CO and CH₄) confirm this analysis.

Finally we discuss the role of the different contributions to the stability and dynamics of the nanotube/nanoparticle interface on the chiral selectivity.



References

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