Exploring epitaxial relationships between catalyst metal nanoparticles and as-grown single-walled carbon nanotubes

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Theoretical [1] and experimental [2] studies have suggested that an epitaxial relationship exists between the catalyst metal nanoparticle and as-grown single-walled carbon nanotube (SWCNT). To further explore this idea, we have recently developed a synthesis technique to prepare compositionally-tuned bimetallic catalysts for SWCNT growth. Systematic variations to the catalyst composition result in changes to the atomic-scale structure. We find that these structural changes result in shifts in the chirality distribution of as-grown SWCNTs [3]. For example, for a series of compositionally-tuned Ni_xFe_{1-x} bimetallic nanoparticles, Ni catalysts produce a relatively wide range of different chiralities with predominantly (9,4) and (7,6) tubes while $Ni_{0.23}Fe_{0.73}$ catalysts produce a relatively narrow range of chiralities with predominantly (8,4) tubes. The experimental results are supported by modeling efforts. Using density functional theory (DFT) calculations, we have shown that nanotubes are stabilized at the nucleation stage by specific structures, *i.e.* compositions, of bimetallic catalyst surfaces [4]. In this talk, we will describe both the experimental and theoretical results in detail, as well as our recent efforts to extend the idea of epitaxial growth to other 1D materials such as semiconductor nanowires.

References

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