

MAR10-2009-001147

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Chirality selection during Catalytic Nucleation of Carbon Nanotubes

JOHN ROBERTSON, Cambridge University

We study the possibility of chirality selection during the catalytic chemical vapor deposition (CVD) of a Single-Walled Carbon Nanotubes (SWNT) by density functional simulations. When nanotubes grow by root growth, the tube's chirality is fixed at nucleation by the chirality of the initial cap that nucleates on the catalyst cluster surface. We previously studied the energies of caps of different chiralities on a flat, fixed Ni(111) layer [1]. We now consider different caps binding to various planes and apices of a 55 atom cluster of Fe and Ni. Firstly, we find that the caps bind more strongly to these nucleation sites than to the flat (111) layer. A second point is that the cap causes considerable distortion of the metal cluster, while the caps themselves are relatively undistorted. This is because C-C bonds are stronger than metal-metal bonds. Of the three high symmetry nucleation sites on the Fe cluster, the binding of (6,5) and (7,5) caps to the pyramidal corner is 2 eV per cap stronger on average than on other sites. Binding energies also depend on the cap diameter, this explains why the pyramid site is less stable for certain caps. For the Ni cluster, there is a strong preference to the zigzag and chiral caps; binding energies for these two caps are generally greater than for armchair caps by 2.5 eV per cap. Lastly, there is strong segregation of carbon atoms to the outside of the cluster, with little dissolution into cluster.

[1] S Reich, L Li, J Robertson, Chem Phys Lett 421 469 (2006)