Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Interplay of Wetting and Elasticity in the Nucleation of Carbon Nanotubes DMITRI SCHEBARCHOV, SHAUN C. HENDY, Industrial Research Ltd., ELIF ERTEKIN, Univerity of Illinois, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Controlling the structure of single-walled carbon nanotubes during synthesis is one of the outstanding challenges of nanoscale science. Some degree of control has been demonstrated through catalytic synthesis, where the interaction with the catalyst is believed to play a key role, but the exact mechanisms leading to preferential growth remain unclear. Here we report on the development of a model that focuses on the lift-off of carbon nanotube caps after nucleation. We test the model using atomistic molecular dynamics simulations and discuss the implications of the model for understanding growth processes that may control chirality. We illustrate the role of the competition between cap strain energy and adhesive forces in the lifting of these caps from the catalyst surface prior to elongation. We show that, given a particular cap structure, there is a lower bound on the catalyst size from which the cap can lift. This lower bound explains the mismatch between nanotube and catalyst diameters observed in experiment. These findings offer new insight into the nucleation of single-walled carbon nanotubes, and they many lead to the design of catalysts that can better control nanotube structure.

Dmitri Schebarchov
Industrial Research Ltd.

Date submitted: 29 Nov 2011 Electronic form version 1.4