Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nonequilibrium statistical mechanics of nanotube nucleation VASILII I. ARTYUKHOV, BORIS I. YAKOBSON, Rice University — A key problem that advanced carbon nanotube applications face is the difficulty of producing pure single-helicity samples. As the elementary processes of nanotube growth are difficult to observe in situ, theoretical understanding of the process is especially important. Direct molecular dynamics simulations offer limited insight due to computational intractability of space- and time-scales involved. We formulated a theory that explains a class of helicity-selective growth experiments, based on classical nucleation theory and crystal growth kinetics.[1] However, a general theory of nanotube growth must also include fast irreversible growth beyond the classical near-equilibrium assumption. Here we construct a coarse-grained model allowing us to rigorously investigate the statistical mechanics of nanotube nucleation and trace how helicity emerges from the global nucleation trajectory ensemble. Importantly, our model can handle the whole range of conditions from perfect reversibility driven by energetics to perfect irreversibility driven by configurational entropy of nanotube caps and edges. Our theory generalizes earlier models in a large advance towards ultimate understanding of helicity-selective synthesis. [1] V.I. Artyukhov, E.S. Penev, and B.I. Yakobson, Nat. Commun. 5, 4892 (2014)

Vasilii Artyukhov
Rice University

Date submitted: 06 Nov 2015 Electronic form version 1.4