Nucleation and growth of carbon nanotubes are driven by the dynamics of their edge

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In classical crystal growth, the interaction of the growing object with its support and the energies of the different facets determine the growth mode and the resulting crystalline structures. The synthesis of carbon nanotubes by chemical vapor deposition poses somewhat similar yet more complex issues. The catalytic particle is both a support and a reactive interface with the growing tube, and many properties are altered because of the nanometric size of the objects.

In this context, we have identified different growth modes driven by the thermodynamic properties of the interface [1, 2] and developed a model of the interface [3], emphasizing the importance of the configurational entropy of the nanotube edge to stabilize chiral tubes and to account for the temperature dependence of tube helicity distributions. This simple model is pushed further to account for more general interface structures and kinetic Monte Carlo (KMC) simulations are developed [4] to study the growth mechanisms and kinetics, and analyze growth rates in relation with the chiral selectivity of the synthesis.

We also discuss new *in situ* measurements of individual CNT growth rates by homodyne polarization microscopy [5] with better temporal and statistical resolution than previous studies [6]. The growth kinetics are surprisingly complex and exhibit instabilities characterized by stochastic alternations of growth, etching, stops and sometimes restarts. These events occur with or without changes in the structure of the single-walled nanotube. We study the latter case, propose a simple modeling and KMC simulations, thus shedding new light on the role of the tube/catalyst interface dynamics for both thermodynamic and kinetic aspects of the growth.

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