

Abstract Submitted
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Initial Stage of Growth of Single-Wall Carbon Nanotubes: Modeling and Simulations¹ I. CHAUDHURI, M. YU, C. S. JAYANTHI, S. Y. WU, University Of Louisville — Through a careful modeling of interactions, collisions, and the catalytic behavior, one can obtain important information about the initial stage of growth of single-wall carbon nanotubes (SWCNTs), where a state-of-the-art semi-empirical Hamiltonian [Phys. Rev. B, **74**, 155408 (2006)] is used to model the interaction between carbon atoms. The metal catalyst forming a supersaturated metal-alloy droplet is represented by a jellium, and the effect of collisions between the carbon atoms and the catalyst is captured by charge transfers between the jellium and the carbon. Starting from carbon clusters in different initial configurations (*e.g.*, random structures, cage structures, bulk-cut spherical clusters, *etc.*), we anneal them to different temperatures. These simulations are performed with clusters placed in the jellium as well as in vacuum. We find that, in the presence of jellium, and for an optimal charge transfer of $\sim 0.2e$, open cage structures (and some elongated cage structures) are formed, which may be viewed as precursors to the growth of SWCNTs. We will also discuss the implications of a spherical boundary on the nucleation of a SWCNT.

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