

### **331b Effects of Substrate, Temperature, and Pressure on Catalyzed Swnt Growth Stages**

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Based on molecular dynamics simulations using a reactive force field, we have proposed<sup>1</sup> that the catalyzed growth stages of SWNTs include carbon dissolution, carbon precipitation as chains, generation of fullerene structures, cap formation, and finally cap elongation into nanotube. Here we discuss these growth stages when the nanocatalyst is attached to the substrate. Also the effects of density and temperature are analyzed and the time scale of our calculations is compared with that of experiments. Preliminary results on the possible reasons by which catalyzed processes may yield selectivity toward specific chiralities are presented.

1J. Zhao, A. Martinez-Limia, and P. B. Balbuena, *Nanotechnology*, in press.