Mechanism of Transition Metal Catalyzed Growth of Single-Wall Carbon Nanotubes

Wei-Qiao Deng, Xin Xu, Jianwei Che, Tahir Cagin, William A. Goddard III

Department of Chemistry, Materials and Process Simulation Center,
California Institute of Technology, Pasadena, CA 91125

Based on ab initio calculation, we study the microscopic mechanism of single-wall carbon nanotubes growth by using the laser vapor deposition technology. A model catalysts, which were previously characterized, says that highly mobile metal catalyst atoms adsorb at the growing edge of the nanotube, where they catalyze the continuing assembly of hexagons from carbon feedstock diffusing along the nanotube wall. [Phys. Rev. Lett. 78 (1997) 2393] However, another model catalysts suggest that the metal catalyst first creates and stabilizes defects in nanotubes and subsequently attracts an incoming carbon atom to anneal the defect. [Phys. Rev. Lett. 85 (2000) 3193] Our calculation results don’t support these mechanisms and provide a new model. It says that metal catalysts atom absorbed at the growth edge will block the adjacent growth site of pentagon and thus avoid the formation of defect. Metal catalysts can also anneal the existed defects. Additionally, our results show that the nanotube growth will terminate in the absence of metal catalysts and also explain why Pt, Nb and Cu are not good catalysts. Based on this new mechanism, we predict the catalytic behaviors for Rh and Pd.
Figure 1. The defect is formed at the absence of metal catalysts.

Figure 2. The metal atoms block adjacent site of pentagon to avoid the defect formation.

Figure 3. Metal catalysts can anneal the formed defect.