Healing Mechanisms During The Growth of Carbon Nanotubes

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Despite considerable progress in synthesis processes, the detailed microscopic mechanisms involved in the growth of carbon nanostructures are still lacking. *In situ* experimental atomic scale investigations are very difficult, whereas computer simulations allow such investigations. Nevertheless, whether the employed method is empirical or semiempirical, all final configurations are plagued by a high concentration of atomic-scale defects. These include, but are not limited to, heptagon-pentagon topological defects, adatoms, and atomic vacancies.

In the present work, we investigate the healing processes of defective carbon nanotubes at atomic scale. We have developed a tight binding (TB) model for nickel and carbon that uses Monte Carlo simulations in the grand canonical ensemble to study the formation of carbon structures (graphene and nanotubes) from a metallic substrate [1, 2]. In particular, we have recently discussed the key role played by metallic atoms in the reconstruction of a defected graphene sheet by annealing defects [3].

We use our TB model to study the evolution at finite temperatures of defected nanotubes. Different lengths and diameters of nanotubes have been investigated at various temperatures ranging from 500 to 3000 K. We have also investigated the role played by the metal catalyst and a vapor of carbon atoms in the healing process. The building up of the tube chirality is analyzed and discussed through electron diffraction patterns. The approach proposed here could help identify individual healing mechanisms during growth that produces perfect tube structures and those favoring a definite chirality [4].

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