Theoretical Study for Microscopic Mechanisms of Carbon Nanotube Growth

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Abstract

We present in this thesis the total energy calculations for the open edge growth mechanisms of carbon nanotubes by the density functional theory and the transferable tight binding model. The energetics of finite-length achiral nanotubes is discussed within the tight binding model at first. Combining the strain energies and the edge formation energies calculated by the tight binding model, we obtain the total energy of the finite-length nanotube as a function of a number of atoms N. It is found that the most stable nanotube at a fixed number N is always the armchair type and the radius of the most stable nanotube increases with increasing N. The adsorption and diffusion of carbon adatoms on the nanotube edge and wall are also investigated using the density functional theory with the local density approximation. It is found that the activation energies of diffusion on the armchair nanotube edge and the zigzag nanotube edge are 2.07 eV and 1.66 eV, respectively. On the other hand, the polygonal defects such as pentagon networks on the nanotube edge which are responsible for the nanotube closure must be annealed out to the hexagon networks to maintain the open edge growth. We discuss annealing out of the polygonal defects by calculations of the activation energies to incorporate the adatom into the polygonal defects. It is found that the adatom on the nanotube wall is incorporated into the polygonal defect more easily than the adatom on the nanotube edge. It is concluded that, in addition to the adatoms on the nanotube edge, the adatoms on the nanotube wall diffusing toward the nanotube edge play an important role of the open edge growth of the nanotubes. Furthermore, we investigate atomic steps on the nanotube edge because the flatness along the edge is not always guaranteed in the open edge growth. The step formation and adsorption of the adatom on the stepped edge are discussed. It is found that the site just below the atomic step becomes a deep sink for the adatoms on the edge, because of the dangling bond generated by the step formation.

List of papers submitted for the requirement of the degree

1. "Atomic and Electronic Structures of Deformed Graphite Sheets", Naokazu Kitamura, Atsushi Oshiyama, and Osamu Sugino: J. Phys. Soc. Jpn. **67** 3976-3984 (1998)
2. "Energetics of Carbon Nanotubes and Adatom Adsorption on Nanotube Edge", Naokazu Kitamura, and Atsushi Oshiyama: J. Phys. Soc. Jpn., submitted.
3. "Open Edge Growth Mechanisms of Single Wall Carbon Nanotubes", Naokazu Kitamura, and Atsushi Oshiyama: J. Phys. Soc. Jpn., submitted.

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