Chapter 5

CONCLUSION

From a viewpoint of the open edge growth of the carbon nanotubes (NTs), the energetics and the kinetics have been investigated. We have discussed at first the energetics of the NT within the TTB model. Although the strain energies of the armchair tubes and the zigzag tubes are almost identical, the edge formation energies of the armchair NT are less than those of the zigzag NT. This is because the DBs on the armchair edge are sufficiently stabilized by the triple bond formation. Combining the strain energy and the edge energy, we have obtained the total energy of the finite-length NT as a function of the number of atoms. It is found that the most stable NTs are always the armchair type and the radius of the most stable NT increases with increasing the number of atoms.

Secondary, the adatom diffusion has been investigated by LDA calculations. It is found that the activation energies of the diffusion on the flat armchair and zigzag edges are 2.07 eV and 1.66 eV, respectively. Furthermore, we have discussed the hexagon network formation and annealing out of the polygonal defects on the NT edge. The pentagon on the armchair edge can be annealed out to the hexagon network by incorporation of the single edge adatom. On the other hand, it is found that the activation energy of 2.47 eV is required to form the heptagon network on the armchair edge by incorporation of the edge adatom. In addition, the heptagon network has the large energy on the armchair edge and this heptagon is easily decomposed into the pentagon plus hexagon networks. It is concluded that the heptagon network hardly exists on the armchair edge. In the case of the zigzag edge, we obtain the relatively large activation energy of 2.80 eV to anneal out the square network to the pentagon network by incorporation of the single edge adatom on the zigzag edge. It is also found that the adjacent pentagons network is energetically more favorable than the hexagon network isolated on the flat zigzag edge. It is expected that the hexagon networks are formed successively along the zigzag edge during the open edge growth.

In addition to the diffusion on the NT edge, the diffusion on the wall edge has been also discussed. While the diffusion on the NT edge corresponds to the diffusion on the usual material surface, the diffusion on the NT wall is specific to the NT. In the open edge growth of the NTs, it is expected that the wall adatom is incorporated into the NT honeycomb lattice at the open edge. Furthermore, the polygonal defects can be annealed out by incorporation of the wall adatom with relatively small

activation energy. In annealing out of the polygonal defects, the wall adatom is always more than double-coordinated and has no deep sink on the NT wall. In the case of the edge adatom diffusion, the structure of the saddle-point where the edge adatom is single-coordinated has relatively high energy. On the other hand, the stable site, such as the seat site of the armchair edge, becomes the deep sink for the edge adatom. Therefore, the activation energy of the diffusion on the edge becomes relatively large. It is concluded that the wall adatoms play an important role in the open edge growth of the NT.

Finally, we have discussed the atomic step on the NT edge. In the case of the armchair NT, it is found that the DB generated by the step formation is the main source of the step formation energy. On the other hand, the adsorptions near the atomic step on the armchair edge are investigated. It is found that the seat site below the step becomes the most stable adsorption site. The large adsorption energy of this site is due to not the increase in the coordination number of the edge adatom but the DB generated by the step formation.

From the viewpoint of the open edge growth of the NT, we have presented the energetics of the finite-length NT and the atomic processes in nanotube growth phenomena. Understandings of these microscopic processes is indispensable to identify the growth mechanism of the NT. We have shown that the behaviors not only of the adatom on the NT edge but also the behaviors of the adatom on the NT wall. It is concluded that the adatom on the NT wall plays an important role to anneal out the polygonal defects on the NT edge which is hindrance of the open edge growth. In this sense, our calculations have revealed one aspect of the growth phenomena, that is, the processes of annealing out the polygonal defects. To identify the growth mechanisms is imperative to open a way of the mass production of the NT. When understandings of the growth mechanism is achieved, the mass and effective production method would be developed. The wide range of the application fields of the NT has been already guaranteed. Therefore, the development of the mass production is greatly expected. Our works in this thesis have presented the fundamentals of the nanotube production. Recent great advance in nanoscale technologies and the computational power for theoretical investigations will clarify the veiled mechanisms in the growth phenomena furthermore and bring about the scientific and industrial applications of NT in no distant future. On the other hand, it is expected that the promising nanoscale science and technology develop remarkably by applications of the NT.