Abstract

Single-walled carbon nanotubes are very important materials. They have exhibited many fascinating electronic, thermal and mechanical properties, with promising technological applications. The conductive properties of these nanotubes depend drastically on the tube radius and chirality of the hexagonal carbon lattice along the tube. A slight change in the winding of the hexagon along the circumference of the tube can transform the tube from a metal into a large-gap semiconductor. The radius of carbon nanotube is a function of two parameters, carbon-carbon bond length and indices (n,m) of the tube. One of the differences between a carbon nanotubes and a graphite sheet is in the value of carbon-carbon bond length.

In this thesis, we investigate a variation of the structural parameters, i.e. the bond lengths and bond angles, of three types of single-walled carbon nanotubes, achiral (i.e., armchair (n,n) and zigzag (n,0) tubes) and chiral (n,m) tubes, from that in the graphite sheet in three situations: first situation refers to the equilibrium structure under ambient condition where we have studied the effect of the tube radius and tube length on these bond lengths and bond angles. In the second situation, we study the behavior of these bond lengths under hydrostatic pressure with circular cross section while the final situation contains the study of the behavior of the bond lengths at shape transition under pressure at which transition from circular to oval cross section takes place. To describe these situations we have divided this thesis in six chapters.

In chapter I, we present the history and major important information of carbon nanotubes such as the types of single-walled carbon, properties, potential applications and review of work done for carbon nanotubes. It also contains the motivation and importance for this work.

In chapter II, we describe the helical and rotational symmetries as a function of one bond length which are used to construct the single-walled nanotubes through the generation of atomic coordinates of carbon atoms on the surface of the seamless cylindrical shape. The description of Tersoff potential, to calculate the potential energy of nanotubes, modification of parameters in Tersoff potential and scaling procedure to check other parameters in this potential are presented in this chapter.
In chapter III, we have presented our numerical procedure which is built on the Tersoff potential and the modification of the helical and rotational symmetries as a function of two bond lengths instead of one. This is applied to investigate the structural parameters, bond lengths and bond angles, of all tubes of three types of single-walled carbon nanotubes in this thesis. The results of all our calculations at ambient condition also present in this chapter. These results include the energetically favourable shape of the cross section for tubes. It also presents the results of the effect of tube radius and tube length on the variation of the bond lengths and bond angles from that of graphitic value for achiral and chiral single-walled nanotubes. For chiral single-walled carbon nanotubes, the study also discusses tubes of several chiralities (tubes in five chiral angles having different radii). Our results indicate that two different bond lengths completely describe the structure of achiral single-walled nanotubes while one bond length describes the structure of chiral tubes. The bond lengths and bond angles in armchair tubes vary with tube radius. The tube length has significant effect on these bond lengths and bond angles. Chiral tubes of special chiral angle show maximum value of bond length. The results of the curvature energy with tube radius and chirality has also presented in this chapter for all these tubes.

Chapter IV contains the investigation of the effect of hydrostatic pressure on bond lengths and bond angles as a function of tube radius and chirality for three types of the single-walled nanotubes assuming that the tubes remain in a circular cross section. In this investigation, we adopt a numerical procedure to get a set of the bond lengths and bond angles under pressure associated with the minimum energy of the tube. There is different behaviour of the bond lengths and bond angles with applied pressure depending on the chirality of the tube. At some critical pressure, the bond lengths become equal. The results of compression under pressure of the macroscopic parameters such as tube radius, tube length, volume and energy of the tubes have also been presented in this chapter. This chapter also contains the elasticity (bulk modulus) under pressure of three types of single-walled nanotubes.

In chapter V, we have recalculated the structure under hydrostatic pressure by relaxing the condition of circular cross section assumed in chapter IV. An analysis regarding the cross-sectional shape transition under pressure at which transition from
circular to oval cross section takes place for armchair$(n,n)$, zigzag $(n,0)$ and chiral $(n,m)$ single-walled carbon nanotubes has been presented. There is a different value of the elliptical aspect ratio at shape transition for armchair, zigzag and chiral tubes. This analysis of the shape transition also includes the effect of the tube radius and chirality on the pressure at which transition to elliptical cross section takes place. We also present in this chapter the elasticity (bulk modulus) at transition pressure for armchair and zigzag nanotubes. The behaviour of the bond lengths and tube radius at transition pressure has also investigated in this chapter for three types of single-walled carbon nanotubes.

Finally, we have summarized and concluded all our results in chapter VI. Important observation regarding differences in the behaviour of the bond lengths for different chirality tubes have been presented in this chapter. Based on the results of the bond lengths behaviour and chirality, the experimental and theoretical researchers are enthused to carry out further work.