Analytical Study of Unit Cell and Molecular Structures of Single Walled Carbon Nanotubes

[1] Devi Dass, [2] Rakesh Prasher, [3] Rakesh Vaid*
[1, 2, 3] Department of Physics and Electronics, University of Jammu, Jammu-180006, India

Abstract:
Recently it has been experimentally confirmed that the chirality of a nanotube controls the speed of its growth, and the armchair nanotube should grow the fastest. Therefore, chirality is an important parameter in designing a carbon nanotube (CNT) and needs to be investigated for the role it plays in the structure of a CNT. In this paper, we have analytically analyzed the unit cell and molecular structures of various single walled carbon nanotubes (SWCNTs) at different values of chirality combinations. The results suggest that total number of unit cells, carbon atoms and hexagons in each structure of SWCNTs are being changed by changing its chirality. A simple and step by step approach has been followed in describing the analytical expressions of overall unit cell structure, molecular structure, chiral angle and diameter of SWCNTs. The analytical formulations have been verified by simulating different SWCNTs at various chirality values. The simulated results match very well with the mathematical results thus validating, both the simulations as well as analytical expressions.

Keywords: chirality, unit cell structure, molecular structure, chiral angle, armchair SWCNT, zigzag SWCNT, chiral SWCNT

1. Introduction

Carbon nanotubes (CNTs) are fourth allotropes of carbon after diamond, graphite and fullerene, with a cylindrical nanostructure consisting of graphene sheet (hexagonal arrangement of carbon atoms) rolled into a seamless cylinder with diameter in the nanometer range i. e. 10^{-9} m. These tubes were first discovered by Sumio Iijima in 1991 [1] and have been constructed with a length-to-diameter ratio up to 132,000,000:1 [2] significantly larger than any other material. CNTs are members of the fullerene structural family, which also includes the spherical buckyballs. Spherical fullerenes are also known as buckyballs, whereas cylindrical ones are known as CNTs or buckytubes. The diameter of a CNT is of the order of a few nanometers (approx. 1/50,000th of the width of an human hair). The chemical bonding of CNTs is composed entirely of sp^2 bonds similar to those of graphite. These bonds, which are stronger than sp^3 bond found in alkanes, provide nanotubes with their unique strength. Moreover, carbon nanotubes naturally align themselves into "ropes" held together by Van Der Waals forces [3]. CNTs can be classified as single walled carbon nanotubes (SWCNTs) and multi walled carbon nanotubes (MWCNTs). SWCNTs consist of single layer of graphite rolled into a cylinder whereas the MWCNTs consist of multi layers of graphite rolled into a cylinder and the distance between two layers is 0.34nm [4 - 5]. SWCNTs with diameters of the order of a nanometer can be excellent conductors [6 - 7]. SWCNTs are formed by rolling a graphene sheet into a cylinder. The way the graphene sheet is rolled is represented by chiral vector or chirality (n, m). If $n = m = l$ where l is an integer then nanotube formed is known as **armchair**, if $n = l$ & $m = 0$, then nanotube formed is known as **zigzag** and if $n = 2l$ & $m = l$, then nanotube formed is known as **chiral**. It means chirality (n, m) of the SWCNTs depends on the value of integer l *e.g.* when $l = 4$, we have (4, 4) armchair SWCNT, (4, 0) zigzag SWCNT and (8, 4) chiral SWCNT.

2. Mathematical Description of SWCNTs

In this section, we have discussed various single walled carbon nanotubes (SWCNTs) analytically so as to understand various parameters associated with their operation. To proceed with the discussion on the geometry of SWCNT [8], let us first consider the geometry of a two dimensional graphene sheet. Figure (1) shows such a sheet where the x- and y- axes are respectively parallel to a so-called armchair direction and a zigzag direction of the sheet. The point O denotes the origin in the sheet. Each of the hexagon corners represents the position of a carbon atom. The structure of SWCNT is specified by a vector called the chiral vector C_h. The chiral vector corresponds to a section of the CNT perpendicular to the tube axis. In figure (1), the unrolled hexagonal lattice of the CNT is shown, in which OB is the direction of the CNT axis, and OA corresponds to the chiral vector C_h. By rolling the graphene sheet so that points O and A coincide (and points B and B' coincide), a paper model of CNT can be constructed. The vector OB defines another vector named translational vector T. The rectangle generated by the chiral vector C_h and translational vector T, i.e. the rectangle $OAB'B$ in figure (1), is called the overall unit cell for the SWCNT. When the overall unit cell is repeated along the length, we get a SWCNT. The chiral vector of the SWCNT is defined as:

$$C_h = na_1 + ma_2 \equiv (n, m) \qquad (1)$$

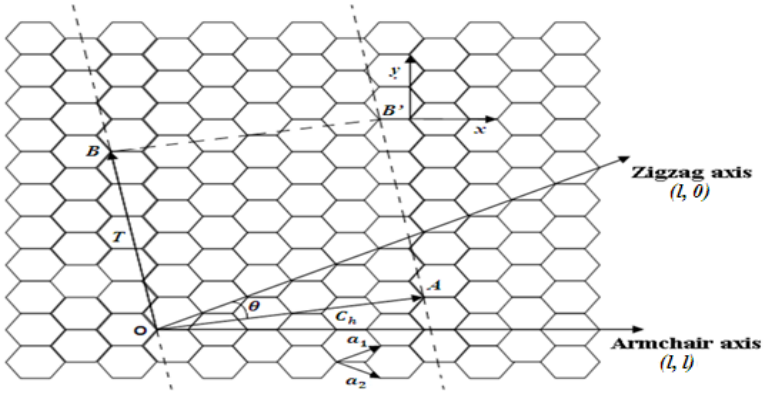

Figure 1. Formation of various SWCNT using chirality (*n*, *m*) [8].

where *n*, *m* are integers *(0≤ |m| ≤ n)* and a_1, a_2 are the unit vectors of the graphene, a_1 specifies the zigzag direction whereas a_2 specifies the armchair direction. In figure (1), a_1 and a_2 can be expressed using the cartesian coordinates (*x*, *y*) as,

$$a_1 = a\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) \quad (2)$$

$$a_2 = a\left(\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right) \quad (3)$$

and the relations:

$$a_1.a_1 = a_2.a_2 = a^2 \quad (4)$$

$$a_1.a_2 = \frac{a^2}{2} \quad (5)$$

where a = 2.46Å is the lattice constant of the graphite. This constant is related to the carbon-carbon bond length $a_{c\text{-}c}$ by

$$a = \sqrt{3}\, a_{c\text{-}c} \quad (6)$$

For graphite, $a_{c\text{-}c}$ = 1.42 Å.

From equations (2) and (3), we observe that the lengths of a_1, a_2, i.e. $|a_1|$, $|a_2|$ are both equal to $\sqrt{3}$ $a_{c\text{-}c}$ = a. By using equations (2) and (3) in equation (1), the chiral vector C_h can be expressed as

$$C_h = \frac{\sqrt{3}}{2} a\,(n + m)\,\hat{x} + \frac{a}{2}(n - m)\,\hat{y} \quad (7)$$

In figure (1), it can be seen that the circumference length of the SWCNT is the length L of the chiral vector which can be obtained from equation (7) as

$$L = |C_h| = a\sqrt{n^2 + m^2 + nm} \quad (8)$$

The angle between the chiral vector C_h and the zigzag axis (or the unit vector a_1) is called chiral angle θ and is defined as by taking the dot product of C_h and a_1, to yield an expression for cos θ:

$$\cos\theta = \frac{a_1.C_h}{|a_1||C_h|} \quad (9)$$

Or by using (2) and (7),

$$\cos\theta = \frac{2n+m}{2\sqrt{n^2+m^2+nm}} \quad (10)$$

Similarly, we have

$$\sin\theta = \frac{|a_1 \times C_h|}{|a_1||C_h|} = \frac{\sqrt{3}\,m}{2\sqrt{n^2+m^2+nm}} \quad (11)$$

From expressions (10) and (11),

$$\tan\theta = \frac{\sin\theta}{\cos\theta} = \frac{\sqrt{3}\,m}{2n+m} \quad (12)$$

Hence, the chiral angle is given by

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}\,m}{2n+m}\right) \quad (13)$$

Rolling the sheet shown in figure (1), so that the end of the chiral vector C_h i.e. the lattice point *A*, coincides with the origin *O* leads to the formation of an (*n*, *m*) SWCNT whose circumference is the length of the chiral vector, and whose diameter is given by

$$d_{(\text{SWCNT})}\,(\text{nm}) = \frac{L}{\pi} = \frac{a}{\pi}\sqrt{n^2 + m^2 + nm}$$

$$= 0.0783\sqrt{n^2 + m^2 + nm} \quad (14)$$

If the chiral vector C_h lies on the zigzag axis i.e. $\theta = 0^o$ and rolling along this axis, a zigzag SWCNT is generated. From equation (13), we see that $\theta = 0^o$ corresponds to $m = 0$ hence a zigzag SWCNT is an (l, 0) SWCNT. If the angle between chiral vector C_h and the zigzag axis is 30^o, it means the chiral vector lies on armchair axis and if the rolling chiral vector along this axis, an armchair SWCNT is generated. From equation (13), we see that $\theta = 30^o$ corresponds to $n = m = l$ and hence an armchair SWCNT is an (l, l) SWCNT. If the chiral vector lies between the zigzag and armchair axis i.e. $0 < \theta < 30^o$ and rolling, a chiral SWCNT is generated. From equation (13), we see that $0 < \theta < 30^o$ corresponds to $n \neq m$ and $m \neq 0$ and hence a chiral SWCNT is like ($2l$, l) SWCNT.

The translational vector T may be expressed in terms of a_1 and a_2 as

$$T = t_1 a_1 + t_2 a_2 \equiv (t_1, t_2) \quad (15)$$

where t_1 and t_2 are integers. The vector T is normal to the chiral vector C_h and thus parallel to the CNT axis. It represents the translation required in the direction of the CNT axis to reach the nearest equivalent lattice point. We know that T is perpendicular to C_h i.e. $T.C_h = 0$ or $(t_1 a_1 + t_2 a_2) \,.\, (n a_1 + n a_2) = 0$. Using equations (4) and (5), the expressions for t_1 & t_2 in terms of n & m are obtained as

$$t_1 = +A\,(2m + n) \quad (16)$$

$$t_2 = -A\,(2n + m) \quad (17)$$

The constant A is determined by the requirement that T specifies the translation to the nearest equivalent lattice point i.e. t_1 and t_2 do not have a common divisor except unity. Thus,

$$A = \frac{1}{d_R} \quad (18)$$

where $d_R = gcd\,(2m + n, 2n + m)$ and gcd stands for greatest common divisor.

Therefore,

$$t_1 = \frac{(2m + n)}{d_R} \quad (19)$$

$$t_2 = \frac{-(2n + m)}{d_R} \quad (20)$$

Hence, from equations (15), (19) & (20), the translational vector T is given by

$$T = \frac{(2m + n)}{d_R} a_1 - \frac{(2n + m)}{d_R} a_2 \quad (21)$$

Or using equations (2) & (3), we get

$$T = \frac{\sqrt{3}a}{2d_R}(m\text{-}n)\,\hat{x} + \frac{3a}{2d_R}(n+m)\,\hat{y} \quad (22)$$

The length of the overall SWCNT unit cell is equal to the magnitude of the translational vector T obtained as

$$L_{\text{(SWCNT unit cell)}} = |T| = \frac{\sqrt{3}a}{d_R}\sqrt{n^2 + m^2 + nm)} \quad (23)$$

The area of the graphene unit cell is given by

$$S_G = |a_1 \times a_2| = \frac{\sqrt{3}a^2}{2} \quad (24)$$

and the area of the overall SWCNT unit cell is given by

$$S_T = |C_h \times T| = \frac{\sqrt{3}a^2(n^2 + m^2 + nm)}{d_R} \quad (25)$$

When the area of the overall SWCNT unit cell S_T is divided by the area of the graphene unit cell S_G, the total number of unit cells in the overall SWCNT unit cell is obtained as a function of n and m as

$$N\,(\text{SWCNT unit cell}) = \frac{S_T}{S_G} = \frac{|C_h \times T|}{|a_1 \times a_2|}$$

$$= \frac{2(n^2 + m^2 + nm)}{d_R} \quad (26)$$

As each unit cell consists of two carbon atoms, therefore, the total number of carbon atoms in the overall SWCNT unit cell can be calculated as

$$N_T\,(\text{SWCNT unit cell}) = 2 \times N\,(\text{SWCNT unit cell})$$

$$= \frac{4(n^2 + m^2 + nm)}{d_R} \quad (27)$$

3. Results and Discussion

In this section, we have discussed various simulation results such as overall unit cell structures and molecular structures for various types of SWCNTs obtained using CNTBands [9] simulation tool and verified analytically.

3.1 Results of Armchair SWCNT

In general, an armchair SWCNT has chirality (*n*, *m*) = (*l*, *l*) where *l* is an integer. The values of *l* are chosen from 1 to 20, so, we have (*n*, *m*) = (1, 1) to (20, 20), and all other parameters are fixed i.e. carbon-carbon spacing = 1.42Å = 0.142nm, tight binding energy = 3eV, and length in 3D view = 50Å = 5nm. By using these parameters, the following results have been obtained.

3.1.1 Overall unit cell structures of armchair SWCNT

The overall unit cell structures of armchair SWCNT for different values of chirality are shown in figure (2).

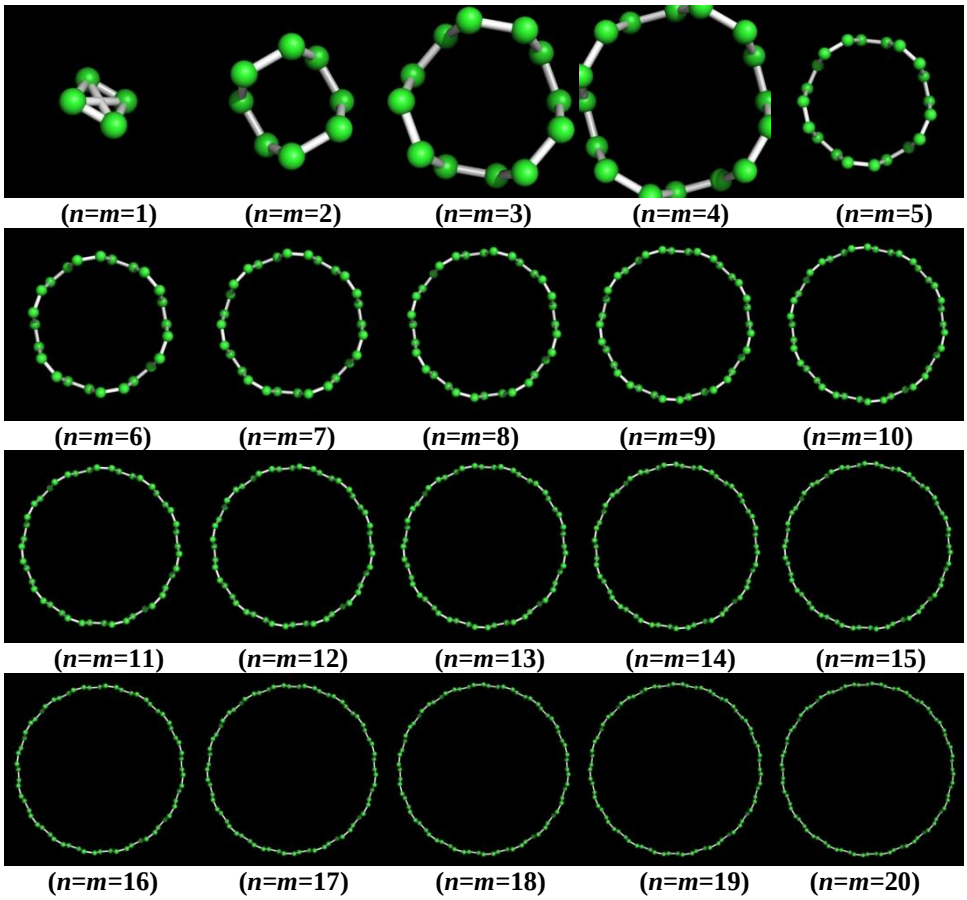

Figure 2. Overall unit cell structures of armchair SWCNT for different values of chirality upto *n*=*m*=20.

In figure (2), each green sphere denotes a carbon atom and white stick denote the bonding between two carbon atoms. A unit cell is a smallest group of atoms and in figure (2), the smallest group consists of two carbon atoms. So, a unit cell consists of two carbon atoms. It has been observed that the total number of unit cells in the overall unit cell structure of armchair SWCNT is increased by 2 as the value of *l* is increased by 1 in its chirality (*n* = *m* = *l*). As each unit cell consists of two carbon atoms, hence, with the increase in the value of integer *l* by 1 of the chirality (*n* = *m* = *l*) of armchair SWCNT, the total number of carbon atoms in its overall unit cell structure is increased by 4. Also, analytically from equation (26), the total number of unit cells in the overall armchair SWCNT unit cell structure is given by:

$$N\,(\text{armchair SWCNT unit cell}) = \frac{2(n^2+m^2+nm)}{d_R} = \frac{2(l^2+l^2+l^2)}{3l} = \frac{6l^2}{3l} = 2l.$$

Thus, analytically, we can say that with the increase in the value of *l* by 1 in the chirality (*n* = *m* = *l*) of armchair SWCNT, the total number of unit cells in its overall unit cell structure is increased by 2. Similarly, from equation (27), the total number of carbon atoms in the overall armchair SWCNT unit cell structure is given by:

$$N_T\,(\text{armchair SWCNT unit cell}) = \frac{4(n^2+m^2+nm)}{d_R} = \frac{4(l^2+l^2+l^2)}{3l} = \frac{12l^2}{3l} = 4l.$$

Hence, we can say that with the increase in the value of *l* by 1 in the chirality (*n* = *m* = *l*) of armchair SWCNT, the total number of carbon atoms in its overall unit cell structure is increased by 4. Therefore, the simulated total number of unit cells and

carbon atoms in the overall unit cell structure of armchair SWCNT are verified analytically. Also, from equation (23) and simulated results, the length of each armchair SWCNT unit cell is 0.246nm.

3.1.2 Molecular structures of armchair SWCNT

The molecular structures of armchair SWCNT for different values of chirality (n, m) are shown in figure (3).

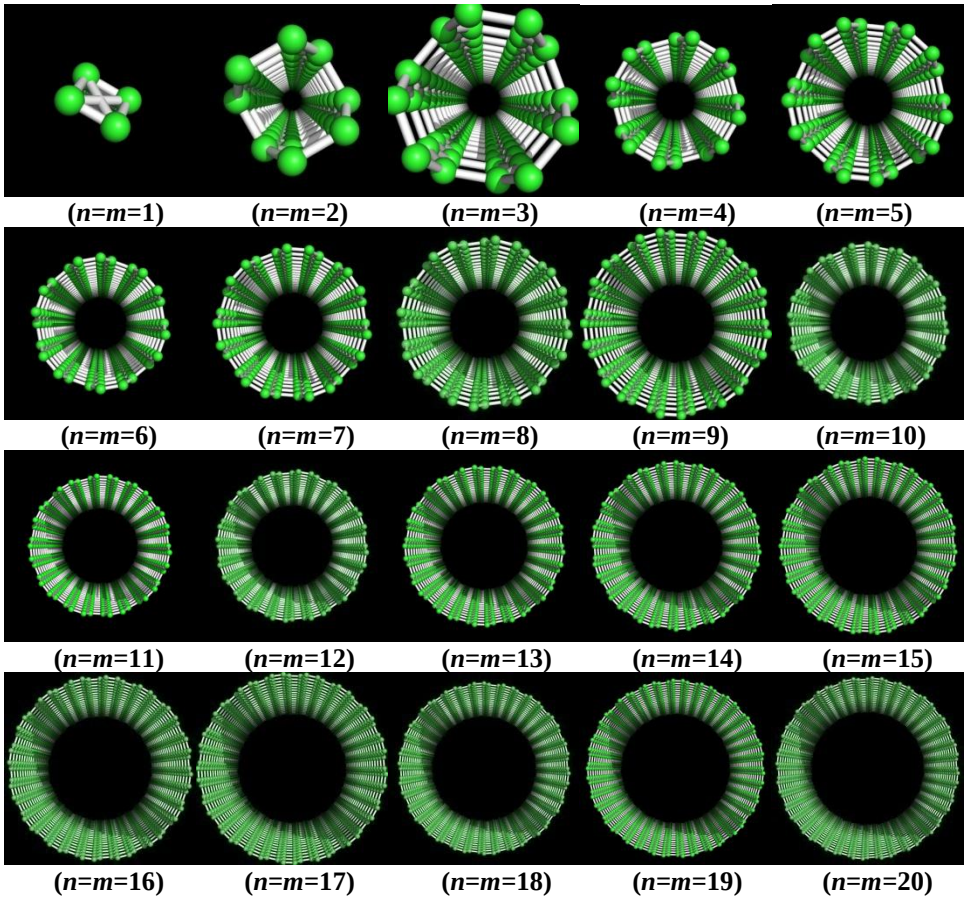

Figure 3. The molecular structures of armchair SWCNT for different values of chirality upto n=m=20.

As per simulation results, the armchair SWCNT unit cell has repeated 5 times per nm length. If we choose the value of length of the armchair SWCNT as 5nm, so, the armchair SWCNT unit cell is repeated 25 times along the length. Therefore, the total number of unit cells in the molecular structure of armchair SWCNT is 25 times the total number of unit cells in its overall unit cell structure i.e.

N(armchair SWCNT) = 25 $\times$ N(armchair SWCNT unit cell) = 2 l $\times$ 25 = 50l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, l) of armchair SWCNT, the total number of unit cells in its molecular structure is increased by 50. As each unit cell consists of two carbon atoms, the total number of carbon atoms in the molecular structure of armchair SWCNT is:

N_T(armchair SWCNT) = 2 $\times$ N(armchair SWCNT) = 2 $\times$ 50l = 100 l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, l) of armchair SWCNT, the total number of carbon atoms in its molecular structure is increased by 100.

The number of hexagons in each ring of armchair molecular structure is l, where l (>1 because hexagons not found in (1, 1) armchair SWCNT) is an integer and the total hexagonal rings in armchair molecular structure = 2 [(Total number of repeated armchair SWCNT unit cell along the length) – 1] = 2 [25 – 1] = 2 $\times$ 24 = 48. Hence, the total number of hexagons in the molecular structure of armchair SWCNT is:

N_{THEX}(armchair SWCNT) = the number of hexagons in each ring of armchair molecular structure $\times$ the total hexagonal rings in armchair molecular structure = l $\times$ 48 = 48 l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, l) of armchair SWCNT, the total number of hexagons in its molecular structure is increased by 48. Also, from equation (13) and simulated results, the chiral angle for armchair SWCNT is 30^o.

3.2 Results of Zigzag SWCNT

In general, a zigzag SWCNT has chirality (n, m) = (l, 0) where l is an integer. The values of l are chosen from 1 to 20, so that (n, m) = (1, 0) to (20, 0), and all other parameters are fixed i.e. carbon-carbon spacing = 1.42Å = 0.142nm, tight binding energy = 3eV, and length in 3D view = 50Å = 5nm. By using these parameters, the following results have been obtained.

3.2.1 Overall unit cell structures of zigzag SWCNT

The overall unit cell structures of zigzag SWCNT for different values of chirality (n, m) are shown in figure (4). It has been observed that the shape of each zigzag SWCNT unit cell is different than the shape of armchair SWCNT unit cell but the total number of unit cells and the carbon atoms in each zigzag SWCNT unit cell is similar to the armchair SWCNT unit cell. Also, analytically from equation (26), the total number of unit cells in the overall zigzag SWCNT unit cell structure is given by:

N (zigzag SWCNT unit cell) = $\frac{2(n^2+m^2+nm)}{d_R} = \frac{2(l^2+0+0)}{l} = \frac{2l^2}{l} = 2l.$

Hence, analytically, we can say that with the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT, the total number of unit cells in its overall unit cell structure is increased by 2. Similarly, from equation (27), the total number of carbon atoms in the overall zigzag SWCNT unit cell structure is given by:

N_T (zigzag SWCNT unit cell) = 2 × N (zigzag SWCNT unit cell) = $\frac{4(n^2+m^2+nm)}{d_R} = \frac{4(l^2+0+0)}{l} = \frac{4l^2}{l} = 4l.$

Hence, analytically, we can say that with the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT, the total number of carbon atoms in its overall unit cell structure is increased by 4. Hence, simulated number of unit cells and carbon atoms in the overall unit cell structure of zigzag SWCNT remains the same as verified analytically. Also, from equation (23) and simulated results, the length of each zigzag SWCNT unit cell is 0.426nm.

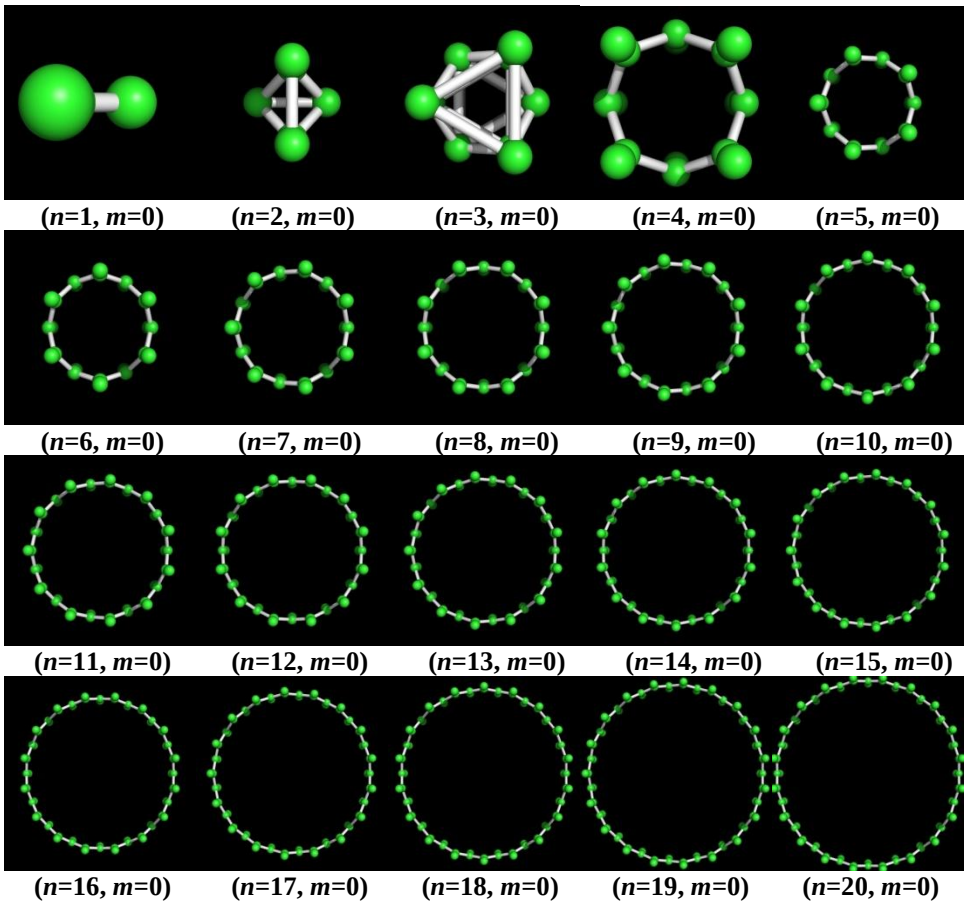

Figure 4. Overall unit cell structures of zigzag SWCNT for different values of chirality upto n=20, m=0.

3.2.2 Molecular structures of zigzag SWCNT

The molecular structures of zigzag SWCNT for different values of chirality (*n*, *m*) are shown in figure (5). As per simulation results, zigzag SWCNT unit cell has been repeated 3 times for 1nm length, 5 times for 2nm length, 8 times for 3nm length, 10 times for 4nm length and 13 times for 5nm length. If we choose length of zigzag SWCNT as 5nm, so, the zigzag SWCNT unit cell is repeated 13 times along the length. Therefore, the total number of unit cells in the molecular structure of zigzag SWCNT is 13 times the total number of unit cells in its overall unit cell structures i.e.

N (zigzag SWCNT) = 13 × N (zigzag SWCNT unit cell) = 2l × 13 = 26l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT, the total number of unit cells in its molecular structure is increased by 26. As each unit cell consists of two carbon atoms, the total number of carbon atoms in the molecular structure of zigzag SWCNT is:

N_T (zigzag SWCNT) = 2 × N (zigzag SWCNT) = 2 × 26l = 52 l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT, the total number of unit cells in its molecular structure is increased by 52.

The number of hexagons in each ring of zigzag molecular structure is l where l is an integer and the total hexagonal rings in zigzag molecular structure = 2 [(Total number of repeated zigzag SWCNT unit cell along the length) – 1] = 2 [13 – 1] = 2 × 12 = 24.

Hence, the total number of hexagons in the molecular structure of zigzag SWCNT is:

$N_{T\,\mathrm{HEX}}$ (zigzag SWCNT) = l × 24 = 24 l.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT, the total number of hexagons in its molecular structure is increased by 24. Also, we can say that the total number of unit cells, carbon atoms, and hexagons in each molecular structure of zigzag SWCNT is approximately half of the total number of unit cells, carbon atoms and hexagon in each molecular structure of armchair SWCNT. Also, from equation (13) and simulated results, the chiral angle for zigzag SWCNT is 0^o.

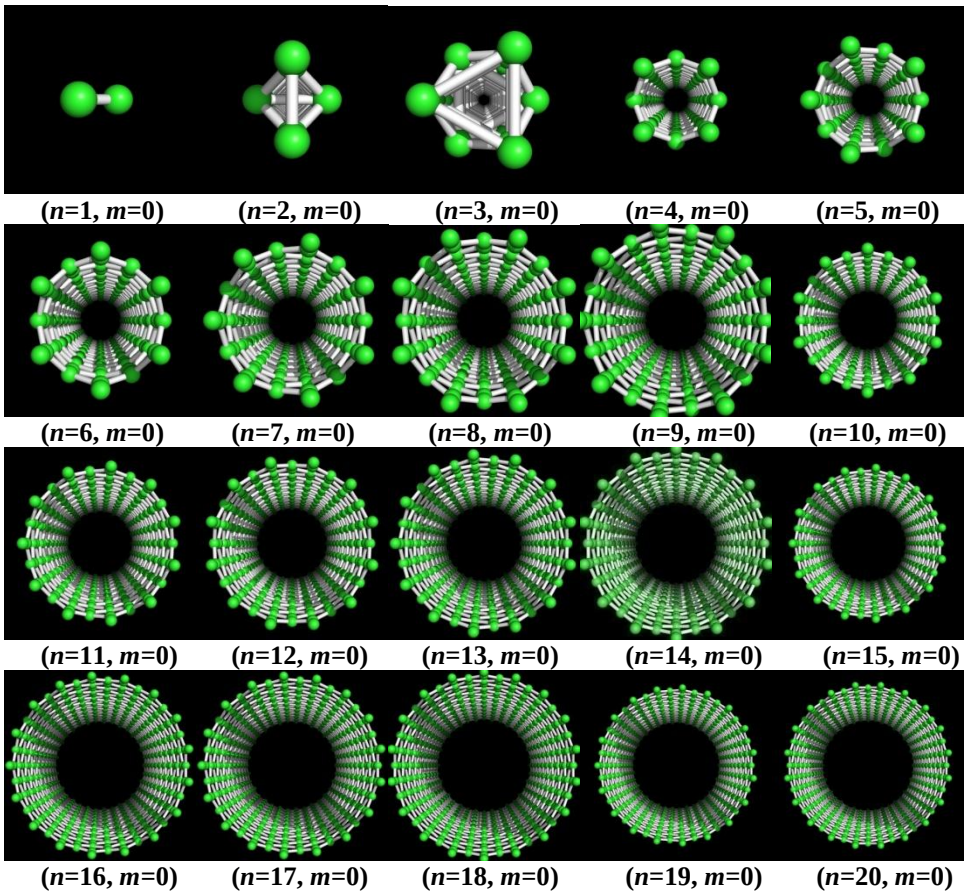

Figure 5. The molecular structures of zigzag SWCNT for different values of chirality upto *n*=20, *m*=0.

3.3 Results of Chiral SWCNT

In general, a chiral SWCNT has chirality (n, m) = ($2l$, l) where l is an integer. The values of l are chosen from 1 to 20, so that (n, m) = (2, 1) to (20, 10), and keeping all other parameters are fixed i.e., carbon-carbon spacing = 1.42Å = 0.142nm, tight binding energy = 3eV, and length in 3D view = 50Å = 5nm. By using these parameters, the following results have been obtained.

3.3.1 Overall unit cell structures of chiral SWCNT

The overall unit cell structures of chiral SWCNT for different values of chirality (n, m) are shown in figure (6).

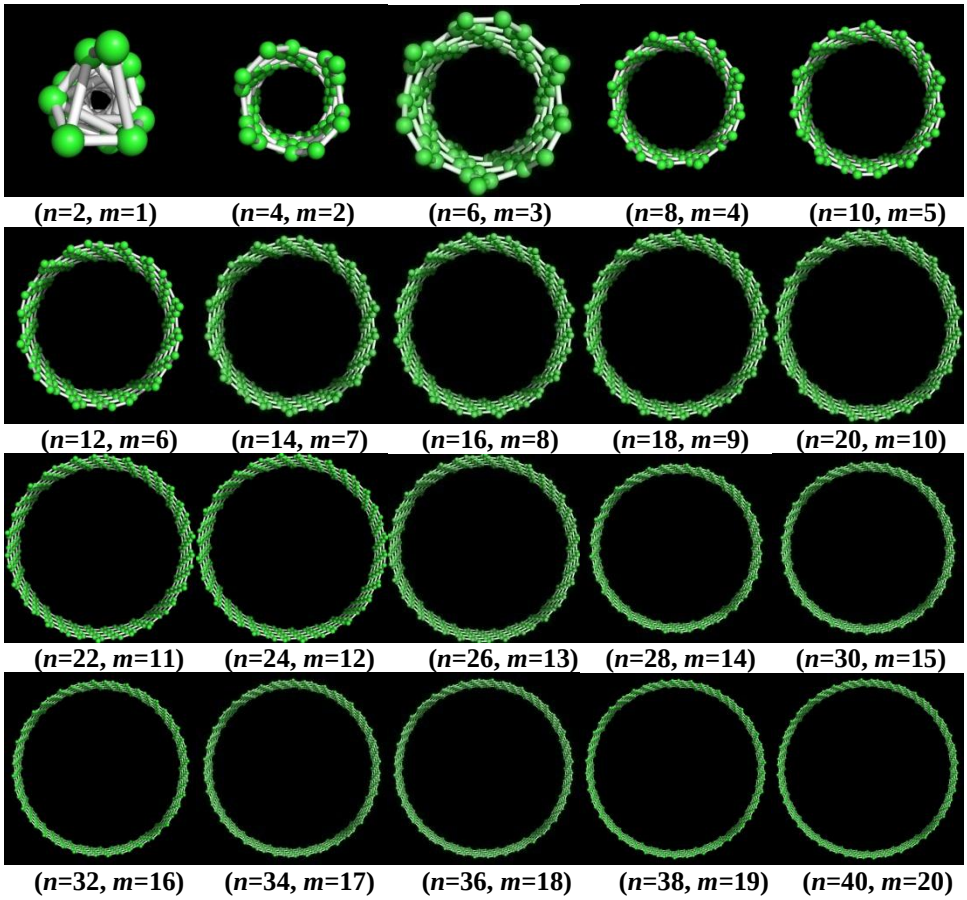

Figure 6. Overall unit cell structures of chiral SWCNT for different values of chirality upto n=40, m=20.

As per simulation results, it has been observed that the total number of unit cells in the overall unit cell structure of chiral SWCNT is increased by 14 as the value of integer l is increased by 1 in its chirality (n, m) = ($2l$, l). As each unit cell consists of two carbon atoms, hence, with the increase in the value of integer l by 1, the total numbers of carbon atoms in the overall unit cell structure of chiral SWCNT is increased by 28. Also, analytically from equation (26), the total number of unit cells in the overall chiral SWCNT unit cell structure is given by:

N (chiral SWCNT unit cell) $= \frac{2(n^2+m^2+nm)}{d_R} = \frac{2(4l^2+l^2+2l^2)}{l} = \frac{14l^2}{l} = 14l.$

Hence, analytically, we can say that with the increase in the value of l by 1 in the chirality (n, m) = ($2l$, l) of chiral SWCNT, the total number of unit cells in its overall unit cell structure is increased by 14. Similarly, from equation (27), the total number of carbon atoms in each zigzag SWCNT unit cell structure is given by:

N_T (chiral SWCNT unit cell) = 2 × N (chiral SWCNT unit cell) $= \frac{4(n^2+m^2+nm)}{d_R} = \frac{4(4l^2+l^2+2l^2)}{l} = \frac{28l^2}{l} = 28l.$

Hence, analytically also, we can say that with the increase in the value of l by 1 in the chirality (n, m) = ($2l$, l) of chiral SWCNT, the total number of carbon atoms in its overall unit cell structure is increased by 28.

Also, as per simulation results, the total number of hexagons in each chiral SWCNT unit cell structure is given by:

N_{THEX} (chiral SWCNT unit cell) = $4m + 3n$ $\quad n, m \geq 2$.

Hence, with the increase in the value of l by 1 in the chirality $(n, m) = (2l, l)$ of chiral SWCNT, the total number of hexagons in its overall unit cell structure is increased by 10. The hexagons are not found in armchair and zigzag SWCNT unit cell structures. Also, from equation (23) and simulated results, the length of each chiral SWCNT unit cell is 1.127 nm. Also, we can say that L (armchair SWCNT unit cell) < L (zigzag SWCNT unit cell) < L (chiral SWCNT unit cell).

3.3.2 Molecular structures of chiral SWCNT

The molecular structures of chiral SWCNT for different values of chirality (n, m) are shown in figure (7).

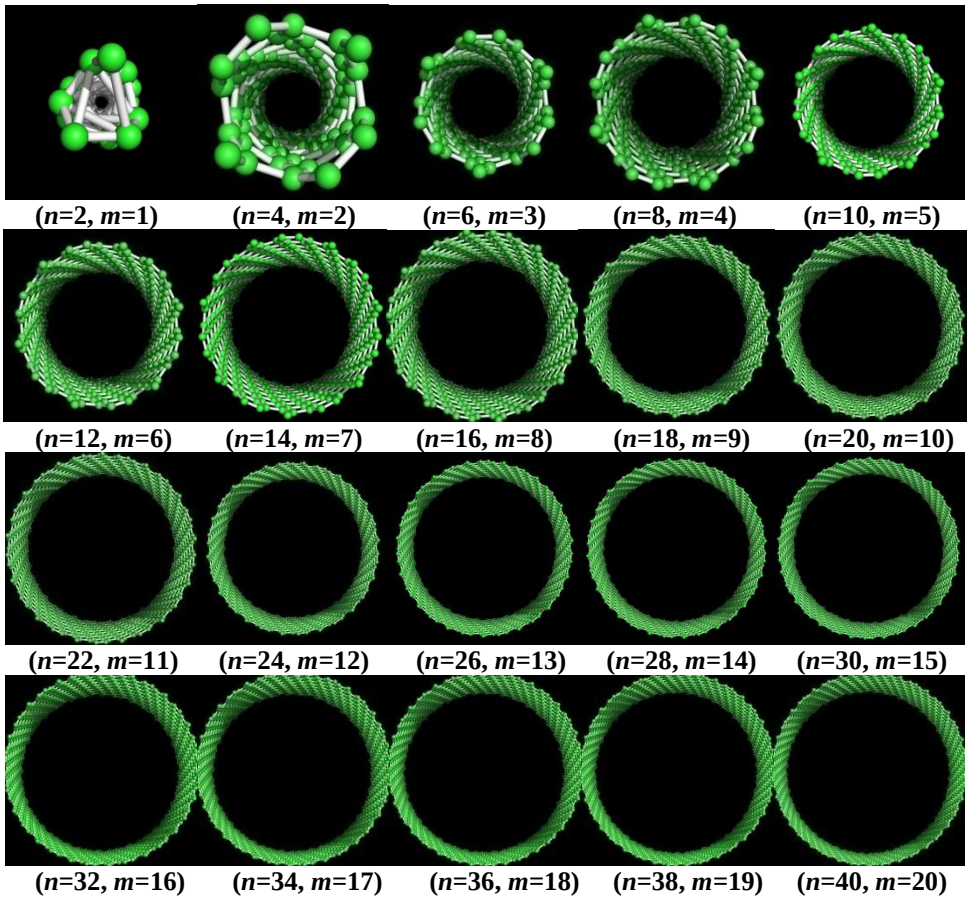

Figure 7. The molecular structures of chiral SWCNT for different values of chirality upto n=40, m=20.

As per simulation results, chiral SWCNT unit cell has been repeated 1 times for 1nm and 2nm length, 2 times for 3nm, 4nm and 5nm length. If we choose length of chiral SWCNT as 5nm, so, the chiral SWCNT unit cell is repeated 2 times along the length. Therefore, the total number of unit cells in the molecular structure of chiral SWCNT is 2 times the total number of unit cells in its overall unit cell structures i.e.

N (chiral SWCNT) = 2 × N (chiral SWCNT unit cell) = 2 × $14l$ = $28l$.

Hence, we can say that with the increase in the value of l by 1 in the chirality $(n, m) = (2l, l)$ of chiral SWCNT, the total number of unit cells in its molecular structure is increased by 28.

As each unit cell consists of two carbon atoms, the total number of carbon atoms in the molecular structure of chiral SWCNT is: N_T(chiral SWCNT) = 2 × N(chiral SWCNT) = 2 × $28l$ = 56 l.

Hence, we can say that with the increase in the value of l by 1 in the chirality $(n, m) = (2l, l)$ of chiral SWCNT, the total numbers of carbon atoms in its molecular structure is increased by 56.

As we know that, chiral SWCNT unit cell has been repeated 2 times along the 5nm length. Hence, the total number of hexagons in the molecular structure of chiral SWCNT can be calculated as:

N_{THEX} (chiral SWCNT) = 8 (n + m) $n, m \geq 2$.

Hence, with the increase in the value of l by 1 in the chirality (n, m) = (2l, l) of chiral SWCNT, the total number of hexagons in its molecular structure is increased by 24. Also, from equation (13) and simulated results, the chiral angle for chiral SWCNT lies between 0^o and 30^o.

A comparison of the total number of unit cells, carbon atoms and hexagons in each overall unit cell structure and molecular structure for all types of SWCNTs with l from 1, 2, 3, 4, 5,----, 20 has been shown in Table 1.

Table 1. Total no. of unit cells, carbon atoms and hexagons in each overall unit cell and molecular structure of three types of SWCNTs for l = 1 to 20 i.e by varying the chirality of SWCNTs.

l	Armchair SWCNT ($n = m = l$)					Zigzag SWCNT ($n = l, m = 0$)					Chiral SWCNT ($n = 2l, m = l$)					
	Overall unit cell structure		Molecular structure			Overall unit cell structure		Molecular structure			Overall unit cell structure			Molecular structure		
	Total no. of unit cells	Total no. of carbon atoms	Total no. of unit cells	Total no. of carbon atoms	Total no. of hexa-gons	Total no. of unit cells	Total no. of carbon atoms	Total no. of unit cells	Total no. of carbon atoms	Total no. of hexa-gons	Total no. of unit cells	Total no. of carbon atoms	Total no. of hexa-gons	Total no. of unit cells	Total no. of carbon atoms	Total no. of hexa-gons
1	2	4	50	100	n.a	2	4	26	52	n.a	14	28	n.a	28	56	n.a
2	4	8	100	200	96	4	8	52	104	48	28	56	20	56	112	48
3	6	12	150	300	144	6	12	78	156	72	42	84	30	84	168	72
4	8	16	200	400	192	8	16	104	208	96	56	112	40	112	224	96
5	10	20	250	500	240	10	20	130	260	120	70	140	50	140	280	120
6	12	24	300	600	288	12	24	156	312	144	84	168	60	168	336	144
7	14	28	350	700	336	14	28	182	364	168	98	196	70	196	392	168
8	16	32	400	800	384	16	32	208	416	192	112	224	80	224	448	192
9	18	36	450	900	432	18	36	234	468	216	126	252	90	252	504	216
10	20	40	500	1000	480	20	40	260	520	240	140	280	100	280	560	240
11	22	44	550	1100	528	22	44	286	572	264	154	308	110	308	616	264
12	24	48	600	1200	576	24	48	312	624	288	168	336	120	336	672	288
13	26	52	650	1300	624	26	52	338	676	312	182	364	130	364	728	312
14	28	56	700	1400	672	28	56	364	728	336	196	392	140	392	784	336
15	30	60	750	1500	720	30	60	390	780	360	210	420	150	420	840	360
16	32	64	800	1600	768	32	64	416	832	384	224	448	160	448	896	384
17	34	68	850	1700	816	34	68	442	884	408	238	476	170	476	952	408
18	36	72	900	1800	864	36	72	468	936	432	252	504	180	504	1008	432
19	38	76	950	1900	912	38	76	494	988	456	266	532	190	532	1064	456
20	40	80	1000	2000	960	40	80	520	1040	480	280	560	200	560	1120	480

To explain the above mentioned values, we have presented the following examples:

Example 1: How many number of unit cells and carbon atoms in the overall unit cell structure of armchair SWCNT for chirality $n = m = 7$. Also, calculate the total number of unit cells, carbon atoms and hexagons in the molecular structure of 5nm long armchair SWCNT for the same chirality.

Solution: An armchair SWCNT has chirality ($n = m = l$). Here $l = 7$.

Therefore, the total number of unit cells in the overall unit cell structure of armchair SWCNT is $2l = 2 \times 7 = 14$.

Total number of carbon atoms in the overall unit cell structure of armchair SWCNT is $4l = 4 \times 7 = 28$.

Total number of unit cells in the molecular structure of 5nm long armchair SWCNT is $50l = 50 \times 7 = 350$.

Total number of carbon atoms in the molecular structure of 5nm long armchair SWCNT is $100l = 100 \times 7 = 700$.

Total number of hexagons in the molecular structure of 5nm long armchair SWCNT is $48l = 48 \times 7 = 336$.

Example 2: How many number of unit cells and carbon atoms in the overall unit cell structure of zigzag SWCNT for chirality $n = 7$, $m = 0$. Also, calculate the total number of unit cells, carbon atoms and hexagons in the molecular structure of 5nm long zigzag SWCNT for the same chirality.

Solution: A zigzag SWCNT has chirality ($n = l, m = 0$). Here $l = 7$.

Therefore, the total number of unit cells in the overall unit cell structure of zigzag SWCNT is $2l = 2 \times 7 = 14$.

Total number of carbon atoms in the overall unit cell structure of zigzag SWCNT is $4l = 4 \times 7 = 28$.

Total number of unit cells in the molecular structure of 5nm long zigzag SWCNT is $26l = 26 \times 7 = 182$.

Total number of carbon atoms in the molecular structure of 5nm long zigzag SWCNT is $52l = 52 \times 7 = 364$.

Total number of hexagons in the molecular structure of 5nm long zigzag SWCNT is $24l = 24 \times 7 = 168$.

Example 3: How many number of unit cells, carbon atoms and hexagons in the overall unit cell structure and molecular structure of 5nm long chiral SWCNT for chirality $n = 14$, $m = 7$.
Solution: A chiral SWCNT has chirality ($n = 2l$, $m = l$). Here $l = 7$.
Therefore, the total number of unit cells in the overall unit cell structure of chiral SWCNT is $14l = 14 \times 7 = 98$.
Total number of carbon atoms in the overall unit cell structure of chiral SWCNT is $28l = 28 \times 7 = 196$.
Total number of hexagons in the overall unit cell structure of 5nm long chiral SWCNT is 70.
Total number of unit cells in the molecular structure of 5nm long chiral SWCNT is $28l = 28 \times 7 = 196$.
Total number of carbon atoms in the molecular structure of 5nm long chiral SWCNT is $56l = 56 \times 7 = 392$.
Total number of hexagons in the molecular structure of 5nm long chiral SWCNT is 168.

4. Conclusions

Based on the analytical formulations and simulation results obtained (see Table 1) using different values of chirality (n, m) in SWCNTs, the following conclusions have been drawn:

For Armchair SWCNT:
With the increase in the value of l by 1 i.e. with the increase in the chirality (n, m) = (l, l) of armchair SWCNT by 1,
(i) Total number of unit cells in its overall unit cell structure is increased by 2.
(ii) Total number of carbon atoms in its overall unit cell structure is increased by 4.
(iii) Total number of unit cells in its molecular structure is increased by 50.
(iv) Total number of carbon atoms in its molecular structure is increased by 100 and
(v) Total number of hexagons in its molecular structure is increased by 48.

For Zigzag SWCNT:
With the increase in the value of l by 1 in the chirality (n, m) = (l, 0) of zigzag SWCNT,
(i) Total number of unit cells and the carbon atoms in its overall unit cell structure is similar than overall armchair unit cell structures.
(ii) Total number of unit cells in its molecular structure is increased by 26.
(iii) Total number of carbon atoms in its molecular structure is increased by 52 and
(iv) Total number of hexagons in its molecular structure is increased by 24 i.e. approximately half than the molecular structure armchair SWCNT.

For Chiral SWCNT:
With the increase in the value of l by 1 in the chirality (n, m) = ($2l$, l) of chiral SWCNT,
(i) Total number of unit cells in its overall unit cell structure is increased by 14.
(ii) Total number of carbon atoms in its overall unit cell structure is increased by 28.
(iii) Total number of hexagons in the overall unit cell structure is increased by 10.
(iv) Total number of unit cells in its molecular structure is increased by 28.
(v) Total number of carbon atoms in its molecular structure is increased by 56 and
(vi) Total number of hexagons in its molecular structure is increased by 24.

References

[1] S. Iijima. Helical Microtubules of Graphitic Carbon. Nature, 354: 56-58, 1991.
[2] X. Wang, Q. Li, J. Xie, Z. Jin, J. Wang, Y. Li, K. Jiang, and S. Fan. Fabrication of Ultralong and Electrically Uniform Single-Walled Carbon Nanotubes on Clean Substrates. Nano Letters, 9: 3137-3141, 2009.
[3] http://en.wikipedia.org/wiki/Carbon_nanotube
[4] R. Saito, G. Dresselhaus and M. Dresselhaus. Physical Properties of Carbon Nanotubes. Imperial College Press, 1998.
[5] M. Dresselhaus, G. Dresselhaus and P. Avouris. Carbon Nanotubes: Synthesis, Structure, Properties and Applications. Springer, 2001.
[6] J. W. Mintmire, B. I. Dunlap, and C. T. White. Are Fullerene Tubules Metallic?. Physical Review Letters, 68: 631-634, 1992.
[7] C. Dekker. Carbon Nanotubes as Molecular Quantum Wires. Physics Today, 52: 22-28, 1999.
[8] H. R. Tabar. Computational Physics of Carbon Nanotubes. Cambridge University press, 2008.
[9] G. Seol, Y. Yoon, J. K. Fodor, J. Guo, A. Matsudaira, D. Kienle, G. Liang, G. Klimeck, M. Lundstrom and A I Saeed. CNTbands. 2010. DOI: 10254/nanohub-r1838.7. Location: https://nanohub.org/tools/cntbands-ext/session/422418.

*Corresponding Author: Dr Rakesh Vaid Email: rakeshvaid@ieee.org