A study of the chirality-related properties of octagonal and dodecagonal carbon nanotubes

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Abstract. The use of carbon nanotubes has grown rapidly over the past decades. The potential of these nanotubes is high and extremely useful in daily life, especially in computer systems and circuits, due to the flexibility of the properties of the nanotubes that can be controlled during their production process. Computer systems rely on the fast conductivity to function. Materials such as graphene, used in carbon nanotubes have proved to be highly conductive materials, more so than the silicon wires used today. This paper explores the possibilities of a new type of carbon nanotube, which has an octagonal lattice instead of a hexagonal lattice of a traditional carbon nanotube, and finds expressions for its basic properties. These properties are compared with that of a traditional hexagonal lattice. This could provide useful applications in the future of physics and computer systems. With the growing need for higher computational power or the design of new materials, a study in such octagonal-shaped carbon nanotubes could prove useful. Dodecagonal-shaped carbon nanotubes are also proposed in this paper with chiral properties equivalent to that of hexagonal carbon nanotubes, which could be explored further as well.

1. Introduction
There is a growing necessity in exploring the properties and applications of carbon nanotubes (CNTs) [1][2][3][4] in our daily life. Single-walled carbon Nanotubes (SWCNTs) are hexagonal sheets of carbon rolled up into a hollow cylinder. The exact point to which the cylinder is rolled up defines the shape and diameter of the nanotube. These points can be measured as a vector, based on the direction when the cylinder is rolled out, which is called the chirality. Changing the chirality of the nanotube can change its electrical and mechanical properties, such as energy band gap, conductivity and strength. The chirality also decides if the tube is a metal or semi-conductor. The flexibility in these properties allows for a wide variety of uses. Although it is still not used at large scales, due to the intense care and high costs required for production, it is hoped that these concerns may be alleviated in the future. This paper explores new octagonal and dodecagonal carbon nanotubes, and their chiral properties are compared with that of hexagonal structures.

1.1 Chirality of a hexagonal SWCNT
The chirality vector is defined as $(n, m)$. In a typical hexagonal-shaped SWCNT, both $n$ and $m$ are integer multiples of the width of a hexagonal unit cell $a$. SWCNTs also have a unique geometry, being a hollow cylinder, capped with half of a fullerene molecule such as the $C_{60}$ buckminsterfullerene molecule.
The chiral angle can be found using the expression, $\theta = \tan^{-1}\left(\frac{m}{n}\right)$, where $m$ and $n$ are integers that scale the vectors of the lattice vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ as shown in Figure 2.

2. Octagonal Lattice for a SWCNT

Considering the geometry and shape of the polygon for the lattice, a hypothetical carbon nanotube with an octagonal arrangement of carbon atoms can be theorized as shown in Figure 2. The geometry of the octagonal sheet consists of 8 sp$^2$ hybridized carbon atoms for each octagon as shown in Figure 3. A continuous interleaved pattern of octagons with squares in between them is necessary to maintain the overall octagonal form.

2.1 Chirality of the octagonal SWCNT

The chiral vector of a SWCNT with an octagonal lattice is given by $\mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2$, where $n$ and $m$ are integers that scale the vectors of the lattice vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ as shown in Figure 2. In the “octagonal” nanotube, C-C bond length is considered as $a_0 = 0.142$ nm. This is also the length of the side of the octagon as shown in Figure 3. The inter-octagonal distance along $\mathbf{r}_1$ is given by $b = 2\delta = a_0 \cot\left(\frac{\pi}{8}\right) = 0.3428$ nm. This inter-cell distance $b$ is larger for the octagonal lattice, than for the hexagonal lattice ($b = 0.2460$ nm). The primitive lattice vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are oriented at an angle of 45° (360/8) relative to each other. The inter-octagonal cell distance in the direction along $\mathbf{r}_2$ is thus, $2\delta \sqrt{2} = b \sqrt{2} = 0.4848$ nm. The properties of such an octagonal SWCNT can be explored and compared with that of a hexagonal SWCNT.

With the inter-octagonal cell distance along $\mathbf{r}_1 = b$, and inter-octagonal cell distance along $\mathbf{r}_2 = b \sqrt{2}$, and considering Figure 2, the circumference of the nanotube can be found using

$$R = b \sqrt{n^2 + (m\sqrt{2})^2 - 2mn\sqrt{2} \cos\left(\frac{3\pi}{4}\right)} = b \sqrt{n^2 + 2m^2 + 2mn}$$ (1)

The diameter of the CNT, $d = \frac{R}{\pi} = \frac{b}{\pi} \sqrt{n^2 + 2m^2 + 2mn} = \frac{0.3428}{\pi} \sqrt{n^2 + 2m^2 + 2mn}$ (2)

The chiral angle can be found using the expression, $\tan \theta = \frac{m}{n + m \sqrt{2} \cos\left(\frac{\pi}{4}\right)} = \frac{m}{n + m}$ (3)
Solving these equations, we get,

Similarly, it can be shown that

The axial translation

2.2 The axial translation vector for the octagonal SWCNT

The axial translation vector \( \mathbf{T} \) is perpendicular to the chiral vector \( \mathbf{R} \).

Let us assume that \( \mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2 \)

Here, \( \mathbf{r}_1 = b \mathbf{i} \) and \( \mathbf{r}_2 = b \sqrt{2} \left[ \left( \frac{1}{\sqrt{2}} \right) \mathbf{i} + \left( \frac{1}{\sqrt{2}} \right) \mathbf{j} \right] = b \mathbf{i} + b \mathbf{j} \)

\[ \Rightarrow b \mathbf{j} = \mathbf{r}_2 - b \mathbf{i} = \mathbf{r}_2 - \mathbf{r}_1 \]

\[ \Rightarrow \mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2 = n b \mathbf{i} + m \left( b \mathbf{i} + b \mathbf{j} \right) = \left( n + m \right) b \mathbf{i} + m b \mathbf{j} \]

Therefore \( \mathbf{T} \) is parallel to \( m b \mathbf{i} - \left( n + m \right) b \mathbf{j} \), or equivalently to \( m \mathbf{r}_1 - \left( n + m \right) \left( \mathbf{r}_2 - \mathbf{r}_1 \right) \).

\[ \Rightarrow \mathbf{T} \text{ is parallel to } \left( n + 2m \right) \mathbf{r}_1 - \left( n + m \right) \mathbf{r}_2 \]

Then we can write \( \mathbf{T} = t_1 \mathbf{r}_1 + t_2 \mathbf{r}_2 \) where \( t_1 = \frac{n+2m}{p} \) and \( t_2 = -\frac{n+m}{p} \),

where \( p \) is the \( \text{gcd} \) of \( n + 2m \) and \( n + m \).

The reciprocal basis vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) are derived from the equations,

\[ \mathbf{r}_1 \cdot \mathbf{b}_1 = 2\pi, \quad \mathbf{r}_1 \cdot \mathbf{b}_2 = 0, \quad \mathbf{r}_2 \cdot \mathbf{b}_2 = 2\pi, \quad \mathbf{r}_2 \cdot \mathbf{b}_1 = 0 \]

which results in \( \mathbf{b}_1 = \frac{2\pi}{b} \left( \mathbf{i} - \mathbf{j} \right) \) and \( \mathbf{b}_2 = \frac{2\pi}{b} \mathbf{j} \)

The octagonal SWCNT reciprocal vectors \( \mathbf{K}_1 \) and \( \mathbf{K}_2 \) are derived from the equations,

\[ \mathbf{R} \cdot \mathbf{K}_1 = 2\pi, \quad \mathbf{R} \cdot \mathbf{K}_2 = 0 \]

\[ \mathbf{T} \cdot \mathbf{K}_2 = 2\pi, \quad \mathbf{T} \cdot \mathbf{K}_1 = 0 \]

Let \( \mathbf{K}_1 = \alpha_1 \mathbf{b}_1 + \beta_1 \mathbf{b}_2 \) and \( \mathbf{K}_2 = \alpha_2 \mathbf{b}_1 + \beta_2 \mathbf{b}_2 \)

Let \( \mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2 \) and \( \mathbf{T} = t_1 \mathbf{r}_1 + t_2 \mathbf{r}_2 \)

Then \( \mathbf{R} \cdot \mathbf{K}_1 = n \alpha_1 \left( \mathbf{r}_1 \cdot \mathbf{b}_1 \right) + m \beta_1 \left( \mathbf{r}_2 \cdot \mathbf{b}_2 \right) = 2\pi \left( n \alpha_1 + m \beta_1 \right) = 2\pi \).

\[ \Rightarrow n \alpha_1 + m \beta_1 = 1 \]

Similarly, it can be shown that \( n \alpha_2 + m \beta_2 = 0 \), \( t_1 \alpha_1 + t_2 \beta_1 = 0 \), \( t_1 \alpha_2 + t_2 \beta_2 = 1 \).

Solving these equations, we get,

\[ \alpha_1 = \frac{n+2m}{n^2+2nm+2m^2}, \quad \beta_1 = \frac{n+2m}{n^2+2nm+2m^2} \]

and

\[ \alpha_2 = \frac{n+2m}{n^2+2nm+2m^2}, \quad \beta_2 = -\frac{n+2m}{n^2+2nm+2m^2} \]

(4)
A summary of the comparison of the properties between the traditional hexagonal CNT and the theoretical octagonal SWCNT is shown in Table 1, and the SWCNT diameters are plotted in Figure 4. The values of the chirality \((n,m)\) are displayed in a decimal format of \(n.m\) on the x-axis in Figure 4.

**Table 1: Comparisons between Hexagonal and Octagonal SWCNTs**

| Feature                     | Hexagonal SWCNT | Octagonal SWCNT |
|-----------------------------|-----------------|-----------------|
| **Geometry**                | Hexagonal lattice | Octagonal lattice |
| **Chiral vector**           | \( \mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2 \) | \( \mathbf{R} = n \mathbf{r}_1 + m \mathbf{r}_2 \) |
| Inter-cell distance along \(r_1\) | 0.2460 nm | 0.3428 nm |
| Inter-cell distance along \(r_2\) | 0.2460 nm | 0.4848 nm |
| Diameter (nm)               | \( \frac{0.2460}{\pi}(\sqrt{n^2 + m^2 + mn}) \) | \( \frac{0.3428}{\pi}(\sqrt{n^2 + 2m^2 + 2nm}) \) |
| Chiral angle                | \( \tan \theta = \frac{m\sqrt{3}}{2n + m} \) | \( \tan \theta = \frac{m}{n + m} \) |
| Axial translation vector \(T\) | \( \mathbf{T} \) is parallel to \((n + 2m) \mathbf{r}_1 - (2n + m) \mathbf{r}_2 \) | \( \mathbf{T} \) is parallel to \((n + 2m) \mathbf{r}_1 - (n + m) \mathbf{r}_2 \) |
| Reciprocal Vectors          |                 |                 |
| \( \mathbf{K}_1 = \alpha_1 \mathbf{b}_1 + \beta_1 \mathbf{b}_2 \) | \( \alpha_1 = \frac{2n + m}{2(n^2 + nm + m^2)} \) | \( \alpha_1 = \frac{n + m}{n^2 + 2nm + 2m^2} \) |
| \( \mathbf{K}_2 = \alpha_2 \mathbf{b}_1 + \beta_2 \mathbf{b}_2 \) | \( \beta_1 = \frac{n + 2m}{2(n^2 + nm + m^2)} \) | \( \beta_1 = \frac{n + 2m}{n^2 + 2nm + 2m^2} \) |
|                             | \( \alpha_2 = \frac{pm}{2(n^2 + nm + m^2)} \) | \( \alpha_2 = \frac{pm}{n^2 + 2nm + 2m^2} \) |
|                             | \( \beta_2 = -\frac{pn}{2(n^2 + nm + m^2)} \) | \( \beta_2 = -\frac{pn}{n^2 + 2nm + 2m^2} \) |

Figure 4: Hexagonal and Octagonal SWCNT diameter plotted vs chirality \((n.m)\)
3. Dodecagonal SWCNTs

One could also consider alternative higher dimensional variants such as a dodecagonal SWCNT as shown in Figure 5, which has dodecagons and triangular shapes interleaved with each other comprised of 12 sp$^2$ hybridized carbon atoms in each dodecagon (this is similar to the interleaving of octagons and squares in the octagonal SWCNT). The inter-dodecagonal distance is given by $a_0 \cot\left(\frac{\pi}{12}\right) = 0.5299$ nm.

If the directions for the $r_1$ and $r_2$ lattice vectors are taken at 60° relative to each other as shown relative to the dotted hexagon in Figure 5, then this has the equivalent chiral properties of a hexagonal lattice with an intercell distance along both directions given by 0.5299 nm so that the results for a dodecagonal SWCNT are merely a scaled version of the results for a hexagonal SWCNT as listed in Table 1 (replacing 0.2460 nm by 0.5299 nm). An alternate modeling could be explored if the directions for the $r_1$ and $r_2$ lattice vectors are taken at 30° relative to each other as depicted in Figure 5.

It is possible that such structures can have interesting properties which could be explored further. For example, the C-C bonds that make up the triangles in a dodecagonal SWCNT could be expected to have a higher strain compared to the C-C bonds that comprise the squares in the octagonal SWCNT, which in turn could have a higher strain relative to the C-C bonds in the hexagonal SWCNT. In addition, the C-C bonds in the triangles in the dodecagonal SWCNTs could have a higher strain relative to the other bonds in the dodecagonal structure. Likewise, the C-C bonds that make up the squares in an octagonal CNT could be expected to have a higher strain relative to the other C-C bonds in an octagonal SWCNT. A difference in strain across different C-C bonds in the octagonal or dodecagonal structures could result in interesting elastic properties in such structures. It may be possible, for example, that “graphene”-like sheets based on such structures could be used to create a form of biodegradable “plastic”, or new electrical conducting materials or strong materials.

![Figure 5: Dodecagonal SWCNTs](image)

4. Conclusion

An octagonal SWCNT is theorized and its chirality-related properties are studied and compared with that of a hexagonal SWCNT. The interleaved structure with octagons and squares may provide interesting elastic properties and strength if such an octagonal SWCNT is realized in the lab. Electrical, optical and mechanical properties could be studied in the future to understand the feasibility and utility of such a design. Dodecagonal SWCNTs could also be explored in the future in the same vein. As carbon and silicon are in the same group in the periodic table (Group 14), one could explore such dodecagonal or octagonal structures based on silicon atoms as well.

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Appendix:

Standard results for hexagonal SWCNTs collected from the NanoHub [5] CNTbands and CNT Mobility simulations are shown in Figure 6. The band gap energy is plotted against the chirality in Figure 6a. The values of the chirality \((n,m)\) are displayed in a decimal format of \(n.m\) on the x-axis in Figure 6b. The energy band-gap is 0 at points 4.4, 6.0, 6.6, 8.2, 8.8, and 10.4. This is because for all these values, \((n-m)\) is a multiple of 3 (which includes the degenerate case of \(n = m\)). So, these are metallic and are very good conductors. For all other values of chirality \((n, m)\), the realized SWCNT is semi-conducting in nature. Ohm’s law states that \(V = IR\), where \(V\) is the voltage, \(I\) is current and \(R\) is Resistance. In addition, resistance \(R = \rho \frac{L}{A}\), where \(\rho\) is the resistivity of the material, \(L\) is the length of the wire, and \(A\) is the cross-sectional area of the wire. The electrical conductivity, \(\sigma = \frac{1}{\rho} = \frac{L}{AR} = \frac{UL}{AV}\). Thus, if \(L\) and \(A\) are fixed for a given SWCNT structure, and if \(V\) is also fixed, then the electrical conductivity is directly related and proportionate to current, which depends on the energy band gap, there can be a relation discerned between the two. The electrical conductance, \(G = \frac{1}{R} = \frac{\sigma A}{L}\). As SWCNTs are hollow tubes, the electron travels along the axis of the tube and on the surface around the circumference of the tube. Hence, the cross-sectional area can be approximated as \(A \propto \pi d\), where \(d\) is the diameter of the nanotube, so that the conductance is proportional to the chiral diameter. For the plots, the length of the SWCNTs was chosen to be fixed at 4 \(\mu m\). The conductivity \(\sigma\) can vary depend on the SWCNT structure due to energy band gap considerations, so that the conductance is a function of both the chiral diameter and the conductivity. The simulated value of the conductance as the chirality properties were varied for hexagonal SWCNTs is shown in Figure 6b. It is hoped that similar studies can be conducted for the octagonal or dodecagonal SWCNTs as such systems are designed and investigated further.