Casp. J. Eng. Mod. Technol., 1(1) (2024) 45-61

Amol University of Special
Modern Technologies

Caspian Journal of Engineering Modern Technologies
Journal homepage: https://cjemt.ausmt.ac.ir/

Research Article

Study of Electronic Properties of Carbon Nanotubes: a Review

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Paper INFO

Paper history:
Received: 2023-05-28
Accepted: 2023-10-25

Keywords:
Nanotechnology;
Nano Devices;
CNTs;
Electronic Properties.

ABSTRACT

In this review we first examine the main issues of nanotechnology. In particular, in the broad scenario of nanoscale devices, we present a detailed study of Carbon Nanotubes (CNTs), which arouse a growing interest for their unique properties and their versatility.
We study and characterize the electronic properties of carbon nanotubes through the determination of the relationship between structure and electronic characteristics of CNTs.

1. INRODUCTION

Technology can be defined as the set of processes or steps of processing required to manufacture devices and systems of any complexity.

The advance of technology is accompanied by the advance of progress where for **progress** we intend all technological products which allow to do: devices for transportation, home automation, medical applications, computing, graphics, telecommunications, creating new tools to acquire knowledge (research), to educate, and so on.

The advancement of technology is measured by the minimum size that a device can reach because the reduction in the size is associated to an increase of the potential or performance (for example the speed) and applications. As technology advances, the minimum size is reduced up to dimensions of several nanometers.

However, the transition from micro-technologies to the nano scale (or **nanotechnologies**) is not trivial but rich in implications.

Nanotechnologies, in fact, do not mark an evolution but a technological revolution and represent the possible solution to not hinder progress.

It is clear, therefore, that they have a key role in the future of humanity and are therefore the subject of considerable research efforts around the world.

Nanotechnology, however, apply to both electronic and optoelectronic devices that involve numerous disciplines of human knowledge [1-2]:

- Biology: build nano-sensors and manipulators of organic matter (same scale of size)
- Medicine: monitoring of markers for cancer, protein and virus detectors, selective administration of drugs, new materials for plant organs, etc.
- Materials science: increased strength, elasticity, structural and electrical properties
- Information, computing, communications: miniaturization of devices, memories, microcomputers, new calculation algorithms, flexible displays with organic LEDs.

Therefore, to move from current technology (**microelectronics**) to nanotechnologies (**nanoelectronics**) we need to change:

a) **Materials and manufacturing processes**, not only silicon but also:

- compound semiconductors of III-V groups of the periodic table
- new structures called Carbon Nanotubes (CNT)
- molecular structures

b) **Architecture of elementary devices**, i.e. switch from traditional semiconductor junction devices to other types:

- Molecular devices (quantum, electromechanical, photoactive)
- Single-electron transistor (SET)
- Resonant Tunneling Devices (RTDs)
- Quantum Dots (QD) and Quantum Cellar Automata (QCA)

c) **Computational algorithms**: new nanoscale devices work according to the laws of quantum physics and not of classical physics, or are based on molecular transfer phenomena and therefore require new "procedures" or calculation algorithm, such as:

- Tactile Computing (molecular devices)
- Quantum Computing (atomic devices).

In the next section we will first seek to define the limits of progress and the consequent role of nanotechnology to the same progress. It will also provide an overview of the nanotechnology revolution with a nod to the possible applications / implications for everyday life.

2. NANOTECHNOLOGY AND LIMITS OF PROGRESS

In 1965, in an article published in *Electronics* [3], Gordon Moore, Fairchild Semiconductor's Director of R&D and one of the pioneers of the C.I. design, tried to answer to the following question: how quickly can advance the progress, i.e. what can we expect between one or ten or twenty years?

Moore, in fact, defined the ability to miniaturize the elementary devices and, therefore, to integrate them into a single chip, as a measure of the progress. Moreover, he hypothesized that the number of transistors integrated on single chip would double every 12 months.

At the end of the 80s the same Moore corrected this forecast on the basis of data regarding the actual progress made in previous years, assuming that there would have been a doubling of the number of transistors integrated on a single chip every 18 months.

This assumption turned out to be correct for many years, from which the name of **Moore's Law** and researchers of INTEL assert that this law will continue to remain valid for at least about 15 years. This means that the next 18 months we assume an increase equal to what occurred in the previous 37 years.

In 2009 INTEL has realized transistors of the minimum size of 15 nanometers, or much smaller than a virus.

Therefore, if the progress is linked to the ability to miniaturize the elementary devices (transistors), it is necessary to reduce their size.

The ongoing miniaturization has many advantages but also many problems. For example, the increase in the number of transistors per chip is associated with a drastic reduction in prices: about 40 years ago a transistor costs $8. Today with a dollar you can buy about one million transistors (without packaging).

This reduction of costs is the reason of the huge spread in integrated electronics equipment of all kinds, in automobiles, in security systems, in computers but also in electronic keys, in remote controls, in toys, etc., in short, in every day life.

However, as you reduce the size of the devices, uncontrollable physical phenomena are unleashed and, often, they do not respect the laws of classical mechanics. Also the risk of malfunction increases as well as **the overheating of the chip**, placing serious difficulties to the validity of the Moore's law.

It seems clear that it makes no sense to continue to miniaturize devices, or to increase the density of integration, without having valid solutions designed to solve the problem of dissipation of thermal power.

Unfortunately, the heat problem is not the only factor of risk of chip malfunction.

There are, in fact, also:

- Power problems (energy) to be supplied to chips so "rich" of transistors;

- design problems of the tracks on which signals travel in chips, especially synchronism signals (clocks);
- reliability problems for so driven technologies;
- problems due to triggering of second order effects or parasitic phenomena (unwanted and uncontrollable);
- physical limits, i.e. there are sizes which physically is not allowed to get for inherent limitations to the structure of matter.

Furthermore, with the miniaturization, transistors will always be more similar to an atom and, in the future, to a part of the atom, and therefore these devices no longer obey the laws of classical mechanics but those of quantum mechanics.

It follows that the progress is likely to stop or, at least, to slow down, disproving Moore's law.

These are the main reasons why the world research is devoted to the study and development of nanotechnologies that currently represent the only hope for non-stop scientific progress [4].

3. BASIC NANOMETRIC DEVICES

Let us examine very briefly some of the major products of nanotechnology, also hinting at their applications.

3.1. Photonic Band Gap Materials (PBG) and photonic devices [5-9]

These are structures sensitive to optical beams and microwaves and not only to electron beams (in which case we speak of *purely electronic devices*).

In particular Photonic Band Gap crystals, known with the acronym PBG, are materials able to influence light propagation as electrons in semiconductors.

In fact, in a semiconductor the atomic lattice causes the formation of a periodic potential for an electron which spreads through it. This periodicity, with the symmetry of the crystalline lattice, determines the formation of energy band gaps for the electronic states, that are of energy bands forbidden to the spreading electrons.

In photonic crystals, to propagate some light quanta (or photons) a principle similar to what is seen for the semiconductor crystals will be exploited, as the crystalline periodicity is artificially realized by means of alternations of dielectric macroscopic materials.

In accordance with the geometrical characteristics of the photonic crystal this will permit the electromagnetic propagation according to some propagation directions and will prevent the same one according to the others: if this last conditions happens, a bandgap exists or rather an interval of forbidden frequencies exists, i.e. the light propagation is not possible along determined directions.

The most important applications of PBG are:

- waveguides, power splitters, switches (low losses over long distances and in presence of strong bendings);
- optical fibers, monomodal in a wide range of wavelength, with a low core refractive index. Only the modes satisfying the Bragg condition can propagate;
- perfectly reflective mirrors, in particular for LASER cavities walls;

- LED diodes having very high external efficiency (4% without PBG) because only the emission of the transmittable modes occurs. All the emitted energy is then transmitted;
- LASER diodes having low threshold (<100 μA): since the spontaneous emission is suppressed (photons having energy inside the band-gap are not emitted) related losses decrease, the efficiency increases, the dissipated power decreases;
- narrow band filters, for DWDM systems;
- resonant cavities with very high Q-factor;
- biomedical sensing applications based on porous silicon;
- particle physics applications to realize high spectral purity accelerators;
- photonic integrated circuits of small sizes.

3.2. Nano - Biosensors and Biochips

The applications of nanotechnology in the field of sensors are of enormous importance and are candidates for a wide short-term spread, being one of few products of nanotechnology already almost ripe for the market.

One of the leading sectors for this type of applications is the biomedical one. In fact, a DNA biochip, for example, is currently quite widespread in biomedical research to recognize DNA sequences, or to determine the genetic map of a subject and, based on this, to know the propensity to certain diseases (useful in prevention), any latent diseases in place, the subjective reaction to medication (useful for a customized dosage of any medication) and so on.

It is expected that within a decade the DNA chip can be commonly used as much as a thermometer to measure body temperature or one stick of blood glucose levels.

Nanosensors, however, play a determining role also to create new systems (micro-electromechanical systems, known with the acronym **MEMS**), able to integrate on a single chip the potential of an entire chemical analysis laboratory (for this also called **lab on chip**). They would enable to perform blood chemistry analyzes in real time, possibly for domestic use, i.e. without to go to a laboratory for analysis.

These chemical biosensors may also allow the real-time environmental monitoring of invisible pollutants and odorless gas coming from any chemical attack.

3.3. Quantum and Molecular Devices

Quantum devices are born from the need to solve a very difficult problem, due to quantum effects, uncontrollable and harmful, that are born in the manufactured electronic devices at the nanoscale.

The design and technological artifices to solve such problems are sometimes not sufficient to ensure a reliable and stable operation in time and, in addition, they often involve a prohibitive increase of costs.

The basic studies in the field of nanoelectronic devices have turned to the examination of quantum effects intended not only as problems to be solved but also as physical effects that can be used for creating new devices based on the principles of quantum mechanics.

This "revolution" implies a totally new concept, in terms of structure and architecture of the devices.

Therefore, the research in this field has proposed:

- devices based on the tunnel effect, whose dimensions are nanometric;
- devices based on the spin of electrons (the spin is an index of the direction of rotation of an electron around its own axis), belonging to the so-called field of **spintronics**;
- devices based on the capture and release of single electrons by means of "tongs" of potential energy (single-electron transistor, quantum wells, trapping ions devices);
- devices based on the polarization of light: the polarization direction is a measure of how the electric and magnetic fiels are arranged in space with respect to the direction of light propagation.

To study and characterize these devices new calculation algorithms have been proposed, giving rise to **quantum computing**.

One of the most surprising features of quantum computing is the incredible computing power because it allows to implement a real parallelism, i.e. a quantum computer behaves as if millions of current classical computers are working.

However, skepticism about the possibility that quantum computing can soon become a reality is mainly related to several problems such as temperature. In particular, in order to control quantum phenomena, it is necessary to operate at very low temperatures, of the order of few kelvin degrees and this is obviously unthinkable at the moment.

Therefore, together with the quantum electronic devices, as possible alternative, research is also focused on the study of **molecular devices** [10], based i.e. on the use of chains of homogeneous or heterogeneous molecules, which allow to slide in a controlled manner a flow of electrons and therefore a current. These devices fall in the field of **molecular electronics**.

3.4. Carbon NanoTubes

Due to their low dimensionality, Carbon NanoTubes, also known with the acronym **CNTs** (**C**arbon **N**ano**T**ubes), have unique electronic and mechanical properties that make them promising candidates for future nanotechnology applications.

However, to truly harness their potential, it is essential to develop a fundamental understanding of the basic physics that governs their behavior in devices. The current research has shown that the concepts learned from bulk device physics do not simply carry over to nanotube devices, leading to unusual device operation. For example, the properties of bulk metal/semiconductor contacts are usually dominated by Fermi level pinning; in contrast, the quasi-one-dimensional structure of nanotubes leads to a much weaker effect of Fermi level pinning, allowing for tailoring of contacts by metal selection. Similarly, while strain effects in conventional silicon devices have been associated with mobility enhancements, strain in CNTs takes an entirely new perspective, with strain-induced bandgap and conductivity changes.

Therefore, they are studying in a wide range of disciplines ranging from solid state physics, chemistry and biology, without well-defined boundaries.

Moreover, CNTs present a unique opportunity as one of the few systems where atomistic based modelling may reach the experimental device size, thus in principle allowing the experimental testing of computational approaches and computational device design. While similar approaches are under development for nanoscale silicon devices, the much different properties of CNTs require an entirely separate field of research.

In particular CNTs present extraordinary electronic properties, related to the ability to have a metallic or semiconducting behavior in relation to their geometry. Therefore it is fundamental to understand the basic physics that governs their behavior in electronic devices.

This will be studied in depth in the following paragraphs.

4. STRUCTURE OF CNTS

Until the mid-1980's pure solid carbon was thought to exist in only two physical forms: diamond and graphite. Diamond and graphite have different physical structures and properties, although their atoms are both arranged in covalently bonded networks. These two different physical forms of carbon atoms are called allotropes.

In particular, as it is known, a carbon atom has four valence electrons on the orbital 2s and 2p, which can easily interact with each other because of the small energy difference between these orbitals. An electron orbital 2s can be combined with one, two, three 2p orbital electrons giving rise to so-called hybridizations sp, sp^2 and sp^3 respectively. In the case of diamond, the four electrons are regularly coupled with the other carbon atoms electrons, thus forming a tetrahedral structure (sp^3 hybridization). This type of bond is very strong, and that is why the diamond is so hard.

Graphite, however, is able to couple stably only three electrons (sp^2 hybridization), leaving the fourth electron free. Each carbon atom is bonded to the three adjacent carbon atoms by covalent bonds of type σ (that is localized along the interatomic direction), which are on the same plane, with angles between them of 120°. Many atoms all together give rise therefore to a planar structure, called graphene, made of filled hexagons whose vertices are, precisely, the carbon atoms. The fourth electron is located in the orbital type π (metallic bond between the floors), which presents lobes orthogonal to the plane of the graphene sheet. The electronic properties of nanotubes can be studied taking into account the energy dispersion relation for the electrons of the π orbitals.

Figure 1 shows a graphite layer, with all atoms bonded between them.

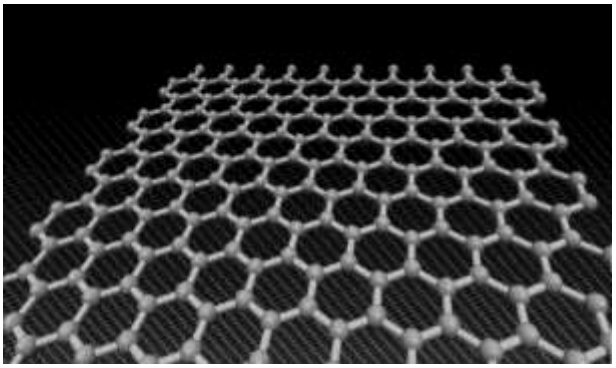

Figure 1. *Planar structure of graphite.*

Graphite is formed by an infinite number of these overlapping layers. As all the electrons which are not coupled, are between two consecutive layers, graphite layers easily slide over each other, making the skin soft and friable. Until 1985 these two forms of crystalline carbon were known.

In 1985 a group of researchers led by Richard Smalley and Robert Curl of Rice University in Houston and Harry Kroto of the University of Sussex made an interesting discovery. They vaporized a sample of graphite with an intense pulse of laser light and used a stream of helium gas to carry the vaporized carbon into a mass spectrometer. The mass spectrum showed peaks corresponding to clusters of carbon atoms, with a particularly strong peak corresponding to molecules composed of 60 carbon atoms, C_{60}.

The fact that C_{60} clusters were so easily formed led the group to propose that a new form or allotrope of carbon had been discovered. It was spherical in shape and formed a ball with 32 faces (12 pentagons and 20 hexagons) similar to a soccer ball ("buckyball") (see Figure 2). This allotrope of carbon was called fullerene, in honor of the architect R. Buckminster Fuller, whose creations, "geodesic domes" (see Figure 3), are similar to the structure of the fullerenes.

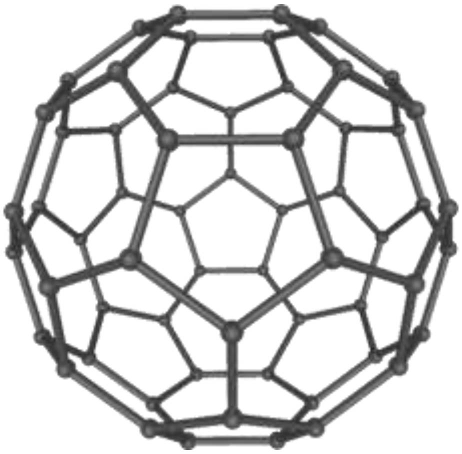

***Figure 2**. C_{60} fullerene, named also "buckyball".*

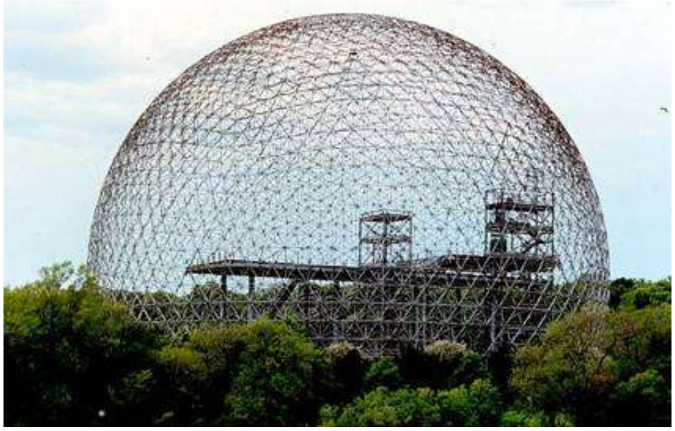

***Figure 3**. Geodesic domes by R. Fuller.*

After this discovery, other related molecules (C_{36}, C_{70}, C_{76} and C_{84}) composed of only carbon atoms were also discovered.

The history of carbon nanotubes has its origins in 1991 with the japanese research Iijima of NEC laboratory in Tsunuba, which demonstrated the possibility of buckyballs bind to form shaped structures tubes closed at the ends, of a few nanometers in diameter. In fact, he observed, casually, the filaments of nanometric dimensions in a residue of soot originated from the vaporization of graphite used for the production of fullerenes. These long, thin structures were called **Carbon NanoTubes** (CNTs).

In particular a CNT is a sheet of hexagonal arranged carbon atoms rolled up in a tube of a few nanometers in diameter, which can be many microns long.

Since the CNT is made up of one or more sheets of graphene rolled up in a tubular structure, the binding in the CNT is nearly identical to that of graphite. The differences in binding are due to the larger inter-shell distance in CNT compared to the interlayer distance of graphite, and the curvature of the graphene sheets.

Figure 4 shows the construction of a graphene sheet, in which carbon atoms are located at each crossing and the lines indicate the chemical bonds, which are derived from sp^2-orbitals [2] [11].

Figure 5 shows the cells and the base vectors of graphene, where a indicates the lattice constant (a = 2,46 Å).

C_h is called **chiral vector** and is given by:

$$C_h = n\bar{a}_1 + m\bar{a}_2$$

being *n* and *m* a pair of integers and $\bar{a}_1$ and $\bar{a}_2$ the lattice vectors, which define a parallelogram constituting the primitive unit cell.

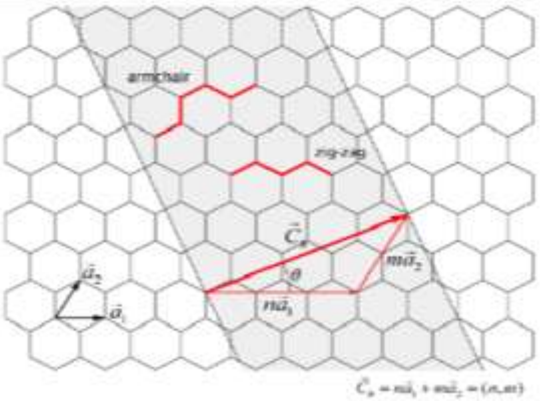

Figure 4*. Graphene sheet indicating the chiral vector.*

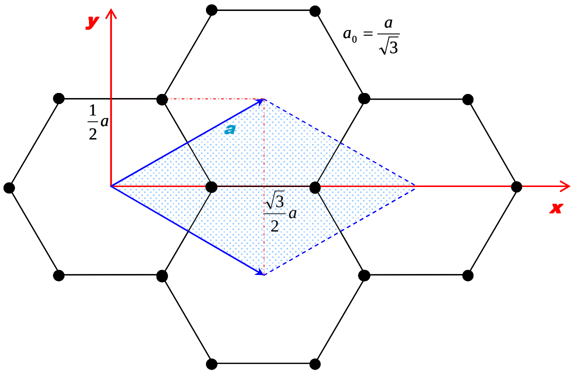

Figure 5*. Cells and base vectors of graphene.*

The angle θ is called **chiral angle**.

In particular we have two particular types of nanotubes (see also Fig. 4):

- those of **armchair type** (n = m, θ = 0°)
- those of **zig-zag type** (n, m = 0, θ = 30°).

For chiral angles 0° <θ < 30°, the nanotubes is named, more generally, as a **chiral type** CNT.

Figure 6 shows these three types of nanotubes.

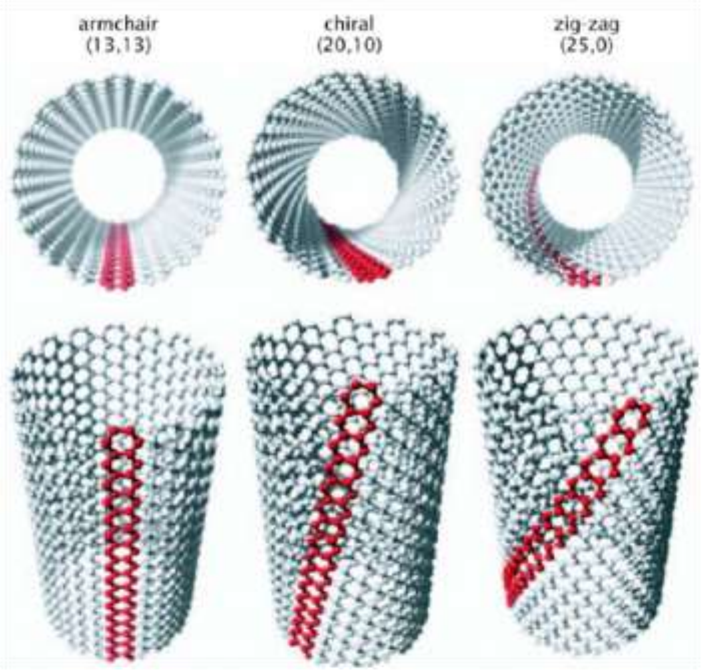

***Figure 6**. Armchair, chiral and zig-zag nanotubes.*

Moreover, referring to Figure 7, the chiral angle θ, as you can easily see, is the angle between the translation vector $\bar{T}$ orthogonal to the chiral vector and the straight line perpendicular to the armchair direction.

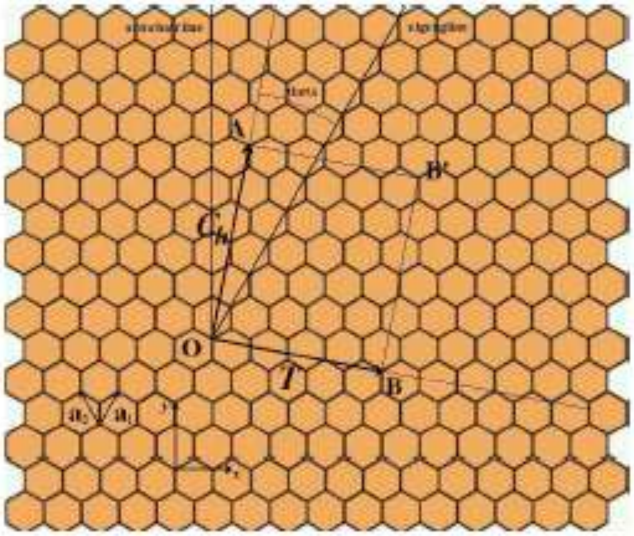

***Figure 7**. Chiral and translation vectors for a nanotube (4, 2).*

The translation vector $\overline{\mathrm{T}}$ describes the distance between two equivalent points of the lattice and is parallel to the axis of the nanotube.

The vectors $\bar{C}_h$ and $\bar{T}$ define the so-called *two-dimensional cell* of the nanotube. In fact, in the winding, the OB side comes to coincide with the AB' side defining the unit cell whose periodic repetition gives rise to the nanotube itself.

Finally, a CNT can be single-wall (SWCNT) or multi-wall (MWCNT).

A SWCNT (Figure 8) is composed by a single cylinder, having a diameter between 0.7 nm and 2 nm. Therefore, the high length/diameter ratio allows to consider it as a one-dimensional structure.

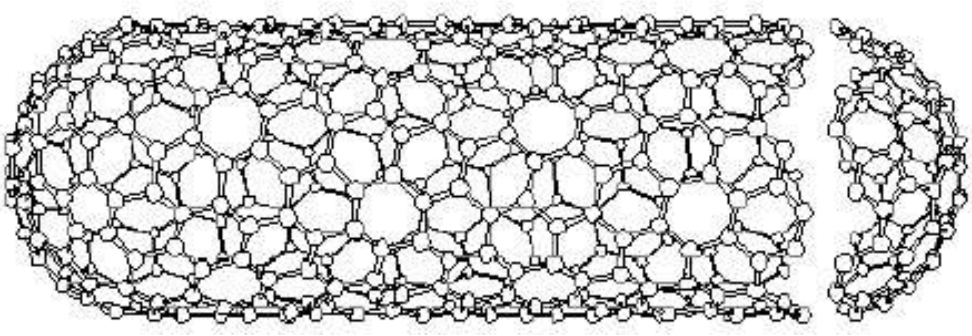

Figure 8. *SWCNT ideal, closed at both ends by two half-fullerenes.*

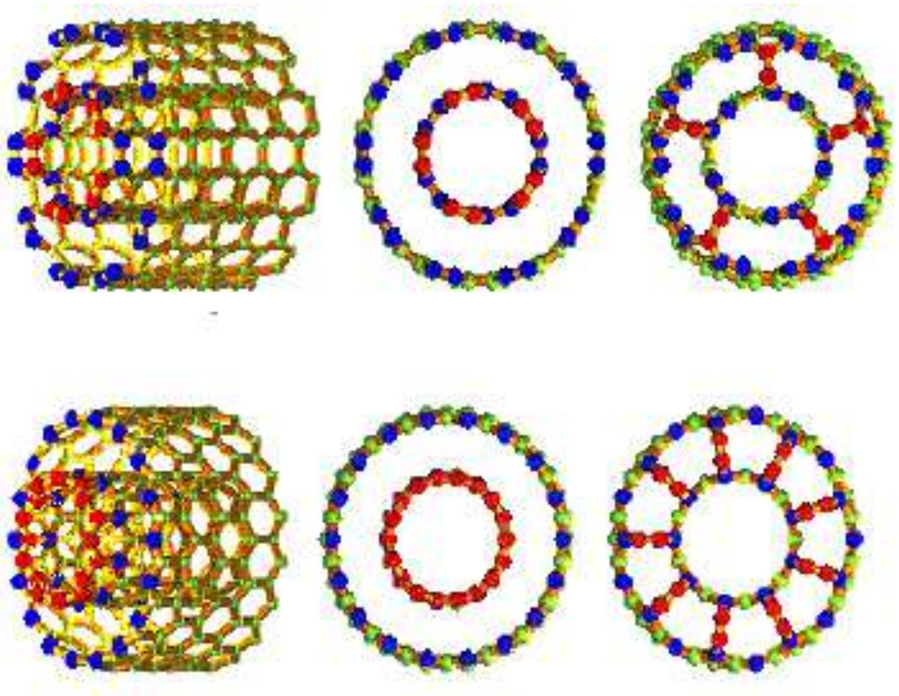

Figure 9. *Types of MWCNT with and without bonds between the walls.*

A MWCNT (Figure 9) is composed of more than one cylinder, having a higher diameter than that of SWCNTs, with possible links between the walls (lip-lip interaction).

As we shall prove, the electronic properties of CNTs depend strongly on the chirality of the nanotube, i.e. on the indices n and m, with $0 \le |m| \le n$ for reasons of symmetry related to the honeycomb lattice: m values outside this range provide the same results.

In fact, depending on their chiral vector, CNTs have either semi-conducting or metallic behavior.

In particular, if *n = m* or *n – m = 3i*, where i is an integer, the nanotube is metallic; in other cases, it shows semi-conducting properties.

Consequently, when the nanotubes are characterized by random values of *n* and *m* we should expect that two-thirds of the nanotube will be semiconductor and the other third metal.

Moreover, we shall demonstrate that the diameter d of the CNT can be calculated by the following equation:

$$d = \left| \frac{\overline{C}_h}{\pi} \right| = \frac{a}{\pi} \sqrt{n^2 + m^2 + nm}$$

and the chiral angle θ by the following equation:

$$\cos\theta = \frac{(n+m)\sqrt{3}}{2\sqrt{n^2 + m^2 + nm}}$$

5. RELATIONSHIP BETWEEN STRUCTURE AND ELECTRONIC PROPERTIES OF CNTs

To study the electronic properties of nanotubes, we start from the analysis of the properties of two-dimensional graphene or graphite sheet.

With reference to Figure 10, the $\bar{a}_1$ and $\bar{a}_2$ lattice vectors can be expressed by the following relations (see also Figure 5):

$$\bar{a}_1 = \left(\frac{\sqrt{3}}{2} a, \frac{a}{2} \right) \qquad \bar{a}_2 = \left(\frac{\sqrt{3}}{2} a, -\frac{a}{2} \right)$$

being a the lattice constant (a = 2,46 Å).

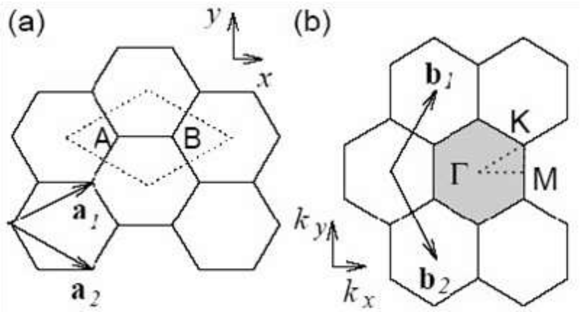

Figure 10*. Direct and reciprocal lattice vectors. The gray hexagon represents the first Brillouin zone of a sheet of graphite. The base cell of the reciprocal lattice is a hexagonal cell rotated of 90°.*

For every cristal structure it is possible to refer to two different lattices: the direct (defined by vectors $\bar{a}_i$) and the reciprocal one, defined by the fundamental vectors $\bar{b}_j$, so that:

$$\left|\bar{b}_i\right| = \frac{2\pi}{\left|\bar{a}_i\right|}$$

or equivalently:

$$\bar{b}_1 = \left(\frac{2\pi}{a\sqrt{3}}, \frac{2\pi}{a} \right) \qquad \bar{b}_2 = \left(\frac{2\pi}{a\sqrt{3}}, \frac{-2\pi}{a} \right)$$

It is worth noting that the vectors in the directed crystal lattice have the dimensions of a length, while those of the reciprocal lattice have the dimensions of the inverse of a length.

Figure 10 shows the vectors of the direct lattice and those of the reciprocal lattice with the respective references.

It is observed that, having chosen as cell for direct lattice the hexagonal cell of Wigner-Seitz, the fundamental cell of the reciprocal lattice constitutes the first Brillouin zone for the graphite sheet.

Note that the band structure of a one-dimensional (1-D) lattice is described in terms of the scalar k = 2π /ʎ. The 1-D Brillouin zones are simply the intervals of k associated to assigned energy bands.

For a 3-D lattice, k becomes a vector in 3-D and the Brillouin zones become volumes. More precisely, a 3-D Brillouin zone is the volume in the k-space which includes all values of k associated with a given energy band.

In order to determine the Brillouin zone relative to the unitary two-dimensional cell in the nanotube, defined by $\bar{C}_h$ and $\bar{T}$, we build the corresponding vectors of the reciprocal lattice, $\bar{G}_C$ and $\bar{G}_T$, respectively parallel to $\bar{C}_h$ and $\bar{T}$, having lengths equal to $\frac{2\pi}{|\bar{T}|}$ and $\frac{2\pi}{|\bar{C}_h|}$, as shown in Figure 11.

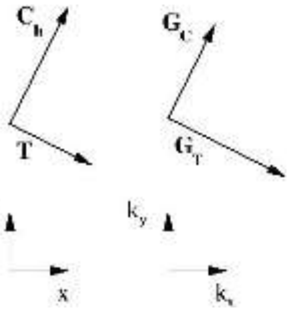

***Figure 11**. Chiral and translation vectors in the direct lattice and their counterparts in the reciprocal lattice.*

The Brillouin zone of the nanotube is given by the rectangle described by $\bar{G}_C$ and $\bar{G}_T$.

When the two-dimensional unit cell of the nanotube is rolled up into a cylindrical shape, the electron is constrained to move in a periodic potential, whose period is C_h.

We intend to justify that there is a discretization of the energy levels along the circumference C_h, corresponding to a discrete set of wave vectors along the vector of the reciprocal lattice $\bar{G}_C$. This gives rise to a series of quantization lines corresponding to the allowable values for the pairs (k_x, k_y).

Moreover, as effect of the stationary condition of the wave associated with the electron, the following relationship has to be satisfied:

$$\bar{k} \cdot \overline{C_h} = 2\pi q$$

where q is an integer and $\bar{k}$ the wave vector.

The electrons are therefore free to move in the direction of the length. In the reciprocal lattice space, we can observe that the quantization lines are spaced by a value:

$$\Delta k = \frac{2\pi}{|\bar{C}_h|} = \frac{2}{d}$$

which depends on the diameter d of the nanotube. Each line corresponds to a one-dimensional conduction channel along the nanotube.

By the relationship that describes the quantization condition along the circumference in dependence on k_x and k_y, we obtain:

$$\left[n\begin{pmatrix} a_{1x} \\ a_{1y} \end{pmatrix} + m\begin{pmatrix} a_{2x} \\ a_{2y} \end{pmatrix} \right] \cdot \begin{pmatrix} k_x \\ k_y \end{pmatrix} = 2\pi q$$

$$\left(na_{1x} + ma_{2x}\right)k_x + \left(na_{1y} + ma_{2y}\right)k_y = 2\pi q.$$

This equation shows a dependence on k_x and k_y and provides the pairs of allowable values in reciprocal space (k_x, k_y): this linear dependence produces the so-called **quantization lines**.

Substituting the expressions of $\bar{a}_1$ and $\bar{a}_2$, we have:

$$\left(n\frac{\sqrt{3}}{2}a+m\frac{\sqrt{3}}{2}a\right)k_x=2\pi q-\left(n\frac{a}{2}+m\left(-\frac{a}{2}\right)\right)k_y$$

$$(n+m)k_x=\frac{4\pi q}{a\sqrt{3}}-\frac{n-m}{\sqrt{3}}k_y$$

$$k_x=\frac{4\pi q}{a(n+m)\sqrt{3}}-\frac{n-m}{\sqrt{3}(n+m)}k_y.$$

The last equation is greatly simplified for:

1. CNT of armchair type (n = m):

$$k_x=\frac{4\pi q}{a(n+m)\sqrt{3}}=\frac{2\pi q}{an\sqrt{3}}$$

2. CNT of zig-zag type (*m* = 0 or, equivalently, *n* = -*m* due to the symmetry properties):

$$k_y=\frac{2\pi q}{an}.$$

Figure 12 shows the wave vectors admissible in relation to the boundary condition for a nanotube of armchair type, zigzag type and chiral type, respectively. The parallel lines represent precisely the allowed vectors $\bar{k}$.

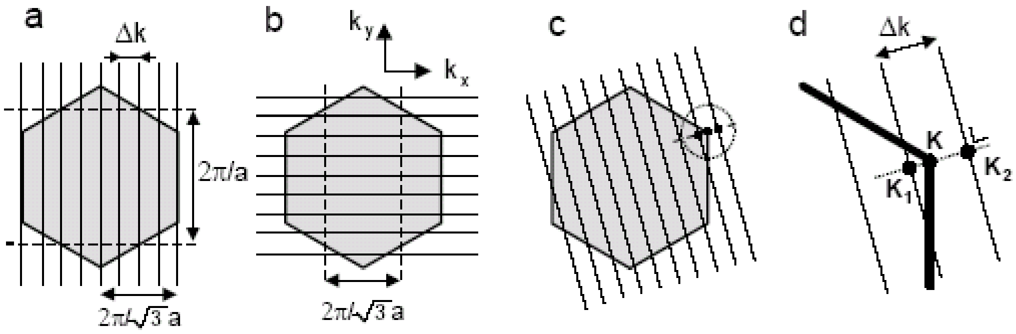

Figure 12. *Wave vectors eligible for nanotube armchair, zigzag and chiral.*

In case of armchair nanotubes, the length of the first Brillouin zone for each permissible line is 2π/a, while for zig-zag nanotubes is $\frac{2\pi}{a\sqrt{3}}$.

We can identify a relationship able to link the (n, m) indexes, the diameter of the nanotube and chiral angle θ. We first observe that:

$$\bar{a}_1\cdot\bar{a}_2=\frac{3a_0^2}{2}\qquad\qquad \bar{a}_1\cdot\bar{a}_1=3a_0^2$$

where $a_0=\frac{a}{\sqrt{3}}=1{,}42\,\text{Å}$ is the length of the covalent bond between two carbon atoms.

Then:

$$d=\frac{|\bar{C}_h|}{\pi}=\frac{\sqrt{\left((n\bar{a}_1+m\bar{a}_2)\cdot(n\bar{a}_1+m\bar{a}_2)\right)}}{\pi}$$

$$=a_0\frac{\sqrt{3}}{\pi}\sqrt{n^2+m^2+nm}=\frac{a}{\pi}\sqrt{n^2+m^2+nm}$$

For the chiral angle, we will have (see also Fig. 4):

$\cos\theta = \cos\left(30^0 - \phi\right)$, where

$$\cos\varphi = \frac{\bar{a}_1 \cdot \bar{C}_h}{\left|a_1\right|\left|\bar{C}_h\right|} = \frac{n + \frac{m}{2}}{\sqrt{n^2 + m^2 + nm}}$$

Therefore:

$$\cos\theta = \frac{(n+m)\sqrt{3}}{2\sqrt{n^2 + m^2 + nm}}$$

The identification of these relationships is important because it allows to go back to the pair of indices (n, m) directly from the values of the diameter and chiral angle, once they are appropriately measured.

For a complete definition of the electronic properties of the nanotubes it is also necessary to define the number N of unit cells of graphene contained in the unit cell of the carbon nanotube. This number is given by the ratio between the area of the graphene cell and the unit cell of the nanotube.

Starting from the conditions:

$$\bar{C}_h \cdot \bar{T} = 0 \quad \text{and} \quad \bar{T} = t_1\bar{a}_1 + t_2\bar{a}_2$$

we can obtain, by developing the scalar product:

$$\bar{C}_h \cdot \bar{T} = 3a_0^2\left(nt_1 + mt_2 + \frac{1}{2}mt_1 + \frac{1}{2}nt_2\right) = 0$$

the following equation:

$$t_1\left(2n+m\right) + t_2\left(2m+n\right) = 0.$$

Since t_1 and t_2 are integers with no common divisors, we have:

$$\bar{T} = \frac{(2m+n)\bar{a}_1}{MCD(2n+m,\, 2m+n)} - \frac{(2n+m)\bar{a}_2}{MCD(2n+m,\, 2m+n)}$$

where MCD is the greatest common divisor between 2n + m and 2m + n.

The area of the unit cell of the nanotube will be:

$$A_{CNT} = \left|\bar{C}_h \times \bar{T}\right| = \frac{2\left|\bar{a}_1 \times \bar{a}_2\right|\left(m^2 + n^2 + nm\right)}{MCD(2n+m,\, 2m+n)}$$

being the area of the graphene cell:

$$A_{graphene} = \left|\bar{a}_1 \times \bar{a}_2\right| = 3a_0^2 sen\frac{\pi}{3} = 3\frac{\sqrt{3}}{2}a_0^2$$

$$N = \frac{A_{CNT}}{A_{graphene}} = \frac{2\left(m^2 + n^2 + nm\right)}{MCD\left(2n+m,\, 2m+n\right)}.$$

In function of N, we derive the constraints of the integer q, introduced in the quantization condition.

As:

$$\bar{k} = k_C\bar{G}_C + k_T\bar{G}_T$$

where:

$\bar{G}_C = \frac{1}{N}\left(-t_2\bar{b}_1 + t_1\bar{b}_2\right)$ and

$\bar{G}_T = \frac{1}{N}\left(m\bar{b}_1 - m\bar{b}_2\right)$ the quantization condition can be reformulated as:

$$k_c = q.$$

Therefore, to avoid the condition of degeneration, it must be:

$$0 \le q \le N - 1$$

This means that there are N discrete values of k in the direction of the chiral vector: in fact $N\bar{G}_C$ may be vector of the reciprocal lattice of the graphene sheet, which, however, may not occur for $0 \le q \le N - 1$, because t_1 and t_2 are prime numbers.

3. CONCLUSION

In this review we have analysed briefly some of the major products of nanotechnology, such as Photonic Band Gap Materials (PBG) and photonic devices, Nano - biosensors and biochips, Quantum and molecular devices.

We have examined in depth Carbon Nanotubes, which have unique electronic and mechanical properties that make them promising candidates for future nanotechnology applications.

However, to truly harness their potential, it is essential to develop a fundamental understanding of the basic physics that governs their behavior in devices. The current research has shown that the concepts learned from bulk device physics do not simply carry over to nanotube devices, leading to unusual device operation.

Moreover, CNTs present a unique opportunity as one of the few systems where atomistic based modelling may reach the experimental device size, thus in principle allowing the experimental testing of computational approaches and computational device design. While similar approaches are under development for nanoscale silicon devices, the much different properties of CNTs require an entirely separate field of research.

Therefore, we have studied the CNTs electronic properties, related to the ability to have a metallic or semiconducting behavior in relation to their geometry, in order to understand the basic physics that governs their behavior in electronic devices.

ACKNOWLEDGEMENT

The author wishes to dedicate this work to Mario Marani and Francesco Marani.

DECLARATIONS

Ethical Approval. The authors declare that there are no animal studies in this work.

Conflict of Interest. The authors declare that they have no conflict of interest.

Author Contributions. First author gave the first idea of investigation, concept and modeling. The methodology has been done by the second author, which also wrote the paper.

Funding. The authors declare that no funds, grants, or other support were received during the preparation of this manuscript.

Data availability. There is no data set used.

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