Mechanisms of Electrical Conductivity in Carbon Nanotubes and Graphene

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INTRODUCTION

In the search for alternative materials to semiconductor materials used commonly in electronics such as silicon, germanium, gallium arsenide, gallium phosphide, etc., researchers around the world have been developing carbon-based materials with ideal electrical properties to operate with high efficiency in nanoelectronics. Carbon nanotubes (CNTs) and graphene represent two technological options for these innovative materials, which can be used either individually, or in composite or hybrid materials as electrical filler. They offer electrical properties such as high electrical conductivity and high dielectric permittivity, which can be tuned by synthesis, doping, functionalization, etc. These qualities can be exploited in applications such as interconnects, electronic devices such as field-effect transistors, batteries, fuel cells, supercapacitors (Yusoff, 2015), electrodes for touch screens (Zheng, 2015), flexible transparent memory circuits, materials for electrostatic discharge (ESD) and electromagnetic interference (EMI) shielding (Vargas-Bernal, 2015c), etc.

This chapter will review the most important electrical transport mechanisms associated with the electrical conductivity of carbon nanotubes and graphene, since these can be used in individual way or within composite or hybrid materials, with the aim of discovering the origin of their extraordinary electrical properties than have been used, are being used, and will be used in diverse technological applications. The effect of a set of technical variables related with electrical behavior of carbon nanotubes and graphene, and associated with the electrical conductivity such as band gap, intrinsic mobility, percolation threshold, electrical conductivity, and dielectric permittivity, are also discussed.

BACKGROUND

Electrical conduction can be defined as the movement of electrical carriers through a transmission medium. A transmission medium is a material substance that transmits or guides through of itself electromagnetic waves. This movement of carriers generates an electrical current in response to an electrical field. Moreover, in each type of material, different mechanisms of electrical conduction are presented. For example, electrons are electrical carriers in metals, and the Ohm's law is the mathematical relationship used to determine the mathematical expression between the electrical current (I) and the applied potential difference (V) between a pair of ends of the material (Bird, 2014):

$$I = \frac{V}{R} = VG, \tag{1}$$

where R and G are electrical resistance and electrical conductance, respectively. Thus, one or more electrons from each atom can move freely within the metal, since they are loosely bound to the atom in the higher level of the valence band. These electrons are incorporated to the conduction band as electrical carriers due to the potential difference, and therefore, an electrical current is generated. An electrical current is a flow of electrical charge carried out regularly by moving electrons through a medium.

Electrical conductivity (σ) also called specific conductance can be defined as the ability of a material for conducting an electrical current. In three-dimensional conductor materials, the electrical conductance can be mathematically expressed as:

$$G = \frac{A}{\rho L} = \frac{Wt}{\rho L} = \frac{Wt\sigma}{L}, \qquad (2)$$

where A is the cross-sectional area, L is the length, W is the width, t is the thickness, and, ρ and σ are electrical resistivity and electrical conductivity of the material, respectively. Two different types of electrical conductivities can be found in materials: surface conductivity and bulk conductivity. Surface conductivity or sheet conductance quantifies the electrical conductance of thin films with uniform thickness nominally. This represents the rate between the electrical conductivity of the material, and the thickness of the thin film. Therefore, it is mathematically expressed as:

$$G_s = \frac{t}{\rho} = \sigma t, \qquad (3)$$

whose units are square per Ohm or Siemen square or denoted by sq/Ω or $\square$/Ω or S·sq or S·$\square$, which is dimensionally equal to an Siemen. Bulk conductance, specific electrical conductance, or volume conductivity (σ) is expressed in units of Siemens per meter (S/m).

Materials can be electrically classified in accordance with their conductivities as conductive, static conductive, or static dissipative (Grady, 2011). The surface conductivity regimes for each are approximately greater than 10^{-4} sq/Ω, $10^{-6}-10^{-4}$ sq/Ω, and 10^{-12}-10^{-6} sq/Ω, respectively. Moreover, the corresponding volume conductivity regimes are > 0.1, $10^{-3}-10^{-1}$, and $10^{-9}-10^{-3}$ S/m. Two applications can be identified in accordance with the value of conductivity: electromagnetic interference (EMI) shielding and electrostatic dissipation (ESD). EMI shielding uses materials with high conductivity, while ESD requires materials with low conductivity.

In materials such as insulators and semiconductors, there is an energy range called forbidden band or band gap, where electron energy states cannot exist between the top of the valence band and the bottom of the conducting band.

MAIN FOCUS OF THE ARTICLE

Carbon nanotubes and graphene has a structure of conjugated system, where a system of connected *p*-orbitals with delocalized electrons in atoms, presents alternating single and multiple bonds, which in general may lower the overall energy of the system and increase stability. Two *p*-orbitals form a π-bond. A π-bond is a covalent chemical bond, where two lobes of one atomic orbital are overlapped to other two lobes of the other atomic orbital involved. Therefore, the π-electrons do not belong to a single bond or atom, but rather to a group of atoms (Jug, 2001). The conjugation can be viewed as the overlap of one *p*-orbital with another across a sigma bond. A simple model of the energy levels can be considered as a quantum mechanical problem of a one-dimensional particle, representing the movement of a π-electron along a long conjugated chain of carbon atoms as found in carbon nanotubes and/or graphene. In this model, the lowest possible absorption energy corresponds to the energy difference between the highest occupied molecular orbital (HOMO), and the lowest unoccupied molecular orbital (LUMO). Almost all electronic transitions in conjugated π-systems are carried from a bonding molecular orbital (MO) to an antibonding MO (π to π*), but electrons from non-bonding Lone pairs (pair of valence electrons that are not shared with another atom) can also be promoted to a π-system MO (n to π*) in charge-transfer complexes. A HOMO to LUMO transition is carried out by an electron if it is allowed by the selection rules for electromagnetic transitions. Thus, the electrical conductivity is guaranteed at using carbon nanotubes and/or

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