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Application of Carbon Nano Tubes for Fabricate Nano Capacitor Including Boron Nitride Dielectric

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Abstract

In this work Nano capacitor was studied by carbon nanotubes electrodes and dielectric of nanotube Boron Nitride. In this research, there are four different configurations which consists of (3,3) & (6,6) & (13,13), (4,4) & (8,8) & (14,14), (5,5) & (10,10) & (15,15), (6,6) & (12,12) & (17,17) and also we calculated total charge electric, potential difference between electrodes, capacity and dielectric constant. All calculations are based on DFT theory and semi empirical method.

Keywords: Boron Nitride nanotube, Capacitor, Carbon nanotube, quantum mechanics

Introduction

Fuel cells, batteries and capacities are systems that are widely used to store energy. Conventional capacitors and batteries have limitations, including short response time. This is due to the movement towards ions in the electrochemical reaction. Recent advances in Nano-scale physics have increased our understanding of the mechanism of energy storage in Nano-materials. Besides reversibility, the effect and high capacity of energy storage and low weight nanostructures, have been considered. Nano structure capacitors have high energy density and are able to store and release the large amounts of lead at speed. Nano capacitors have high to load to transfer rates, long life and short cycle charge compared to batteries which make them useful for a variety of applications [1-4]. Because their nanometer size and their properties such as electrical conductivity, mechanical strength available surface, low resistance and high stability carbon nanotubes are suitable as capacitor electrodes [5]. There are two types of carbon nanotube electrodes 1- bind free [6] 2- binder-enriched [7]. The mentioned types of electrodes are used in electrochemical capacitors [8]. After the discovery of carbon nanotubes in 1991[9], Boron Nitride nanotubes (BNNTs) were synthesized in 1995. There exists sp^2 bonds that cause the strength of these tubes. The predicted elastic modulus for this material is approximately 850 GPa [9]. In some features Boron Nitride nanotubes are better than carbon nanotubes. Theoretical studies have predicted that nanotube Boron Nitride is an insulating material. Its electrical energy gap is about 5/5 eV [10]. These characteristics do not depend on the diameter and chirality of the nanotubes based on conductivity measurements all BNNTs exhibit insulating or semi conducting behavior. Also, BNNTs have more stable chemical properties. For example, they have higher resistance to oxidation at high temperature up to 800^0C. Some of BNNTs that have the complete Nano-crystalline structures can have a thermal resistance of up to 900^0 C. This is while carbon nanotubes are easily in the air at 400^0 C and burn completely at 700^0 C [11]. BNNTs have three different types of configurations, 1-zigzag (n, 0) 2- arm chair (n, n) 3- non chiral (n, m). Depending on the synthesis methods, different configurations of the nanotubes are generated [13-17].

Details of calculation

Figure 1 shows the cross section of a cylindrical capacitor of length l, which consists of two coaxial cylinders in radius (a) and (b) with q charge on each tube. Since $l \gg b$, it is possible to ignore of non -uniformity of the edges.

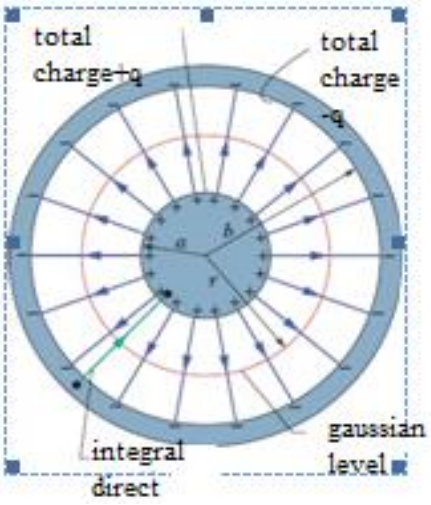

Fig1. Cross section of a cylindrical capacitor

The Gaussian level is selected as a cylinder of length l and radius r and axially with cylinder which includes a central cylinder. There for, the Gaussian level contains the charge in following equation 1.

$$(1)\ q = \varepsilon EA = \varepsilon E\left(2\pi rl\right)$$

'A' is the area of the cross section of the Gaussian side and the flow doesn't pass from the surface of the two cylinders. By solving the above equation, we will have an electric field, equation 2:

$$(2)\quad E = \frac{q}{2\pi rl\,\varepsilon}$$

In the eq 2, $\varepsilon = \kappa\varepsilon_0$, ε_0 is the value of the permittivity for air which is $8/85*10^{-12}$ f/m and K is the permittivity of the dielectric medium used between the two tubes. Also The potential is obtained by the integral, it is as follows 3:

$$(3)\ V = \int_{-}^{+} Eds = \frac{-q}{2\pi\varepsilon l}\int_{b}^{a}\frac{dr}{r} = \frac{q\ln\left(\frac{b}{a}\right)}{2\pi\varepsilon l}$$

dr =ds. By using of the relation c=q/v, capacity is obtained by equation 4:

$$(4)\ c = \frac{2\pi\varepsilon l}{\ln\left(\frac{b}{a}\right)}$$

Theorical model

In this work, the calculations were carried on model. In this model a small capacitor was made by creating an insulating tube of BN between two carbon tubes, for making this model nanotube modeler software was used, figure 2.

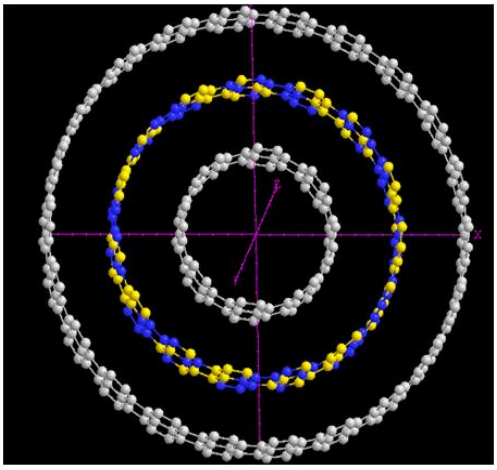

Fig2. Model of Nano capacitor

The calculations were performed by using Gaussian 09 software and the method of DFT and semi empirical method and chelpg and extended Huckel commands and m06-2x. The m06-L, m06-2x and m06-HF are new method hybrid DFT functional method with a good correspondence in non -bonded calculations are useful for calculating the energies of the distances between two coaxial cylinders of radius R_{in}, R_{out} and in the cylindrical capacitor. The lattice constant has been optimized for the atomic coordinate and has done through the minimization of the total energies. For geometries optimizations, all the internal coordinates were relaxed until the Hellmann- Feynman- forces were less than 0.05 angstrom. At each inter tube configuration, a single point calculation is carried out and the total energies are recorded, the resulting sliding rotation energy surface is used for fixing our model in a better position. We used DFT theories with the van der Waals DFT for modeling the exchange – correlation energies of BNNT and CNT. The DZV(double zeta basis set) basis set with polarization orbital was used for nanotube. The charge transfer

and electrostatic potential were calculated via an extended Huckel method. The extended Huckel is a semi empirical method. For a non -covalent interaction, B3LYP cannot to describe Vander Waals interaction [18-19] in capacitor systems by medium rang interactions, such as the interactions of two electrodes and dielectric sheet. Failure of B3LYP and the other functional to describe medium range of exchange and correlation energy correctly, limits their suitability for non bonded distant systems of two electrodes and dielectric in a capacitor. The most recent studies have shown that in exactitude for the medium range exchange energies lead to large systematic errors in the divination of molecular properties [20-24].

Results and discussion

In this studying, BNNT, was chosen as a dielectric because it is an excellent spacer with a lattice constant close to the carbon nanotube (CNT). We specially studied the dielectric properties of CNT/ BNNT/ CNT, the sp^2 hybridized B-N and C-C bonding has the similar properties in mechanics, but their optic and electronic properties are different. Fundamentally the equivalent points result from the close positions of N, B and C in the Mendeleev table, but the different ones result from the heterogeneous atoms. The bonding orbit p of B-N is principally dominated by 2p orbit of N and 2p orbit of B contributes mostly to the anti-bonding orbit p*.

It was considered that the electrodes carry ±q charges from one electrode towards the opposite side. So the initial energy stored in the electrical field between the capacitor tubes is obtained by $E_i=q^2/2c$, one of the fundamental effects in Nano electronics are related to the significant change in the energy when the electrons are transferred into a Nano material such as quantum dot. By letting the electrons tunnel through the insulating tube from the negative terminal to the positive terminal and stored energy is $E_f = (q+\Delta q)^2/2c$. Although the charge is quantized itself, but the charge on the capacitor tubes is polarized and not quantized. The energy cannot stored in the capacitor tubes until a single electron tunnels through the insulator BN tubes from the negative terminal to the positive terminal that energy is $\Delta E= E_f - E_i$, when the quantum well descends below the Fermi level, the electrons start to pour in this quantum well and the excess electrons in the carbon nanotubes become sensitive to charge reveal into the vacuum space of capacitor.

In the Table 1 four different configurations and their diameter are shown. d_1 is diameter of internal carbon nanotube, d_2 is diameter of BNNT and d_3 is diameter of external carbon. The values of the electric charge from $(\left|\Delta q \times 10^{20}\right|)c = \sum q_{out} - q_{in}$ are shown in the table2. Electric charge has Coulomb(c) unit. The potential difference is obtained from equation $\Delta V = \sum (V_{out} - V_{in})$

V_{out} is average potential difference of external electrode and V_{in} is average potential difference of internal electrode, Table2. The q_{out}, q_{in}, V_{out} and V_{in} were obtained from Gaussian program computations.

The following equation is used to calculate the capacity c=q/v, capacity has farad unit, table2. K is calculated by equation 4. The values of K are obtained 5/9 for total configurations.

Conclusion

We studied Four different configurations consists of (3,3) & (6,6) & (13,13), (4,4) & (8,8) & (14,14), (5,5) & (10,10) & (15,15), (6,6) & (12,12) & (17,17). Total charge electric, potential difference between electrodes, capacity and dielectric constant were calculated, Table 2.

BNNT usually can be used as an insulator regardless of its diameter and helicity or the number of walls and dielectric constant of Boron Nitride nanotubes doesn't depend on diameter and configuration. Capacity for four different configurations increased from the increase diameters. These Nano capacitors were sensitive to the existence of molecules inside them and are under the influence of the resulting induced electrostatic field. The structural properties of these Nano capacitors had the ability of transferring charges and electromagnetic current to bonds and the charge transfer along the Nano capacitors, created a regular electromagnetic current around the Nano capacitors. These quantity values exhibited a Gaussian distribution and different expectation values could be referred to each quantized level. It seems that research on such a non -bonded interaction in the carbon Nano tube would be a promising way to cure the chemical and physical properties of carbon compounds and may avail as a starting point for designing electromagnetic Nano systems to be considered in experiments.

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Table1. Four different configurations and their diameter

Nano capacitor CNT/BNNT/CNT	$d_1 *10^{10}$(m)	d_2*10^{10} (m)	$d_3 *10^{10}$ (m)
(3,3)@(6,6)@(13,13)	4/039	8/079	17/504
(4,4)@(8,8)@(14,14)	5/38	10/77	18/85
(5,5)@(10,10)@(15,15)	6/73	13/46	20/197
(6,6)@(12,12)@(17,17)	8/079	16/157	22/89

Table2. The total charge, potential difference and capacity values calculated for different configurations

Nano capacitor CNT/BNNT/CNT	$(\lvert\Delta q\times 10^{20}\rvert)c=\sum q_{out}-q_{in}$	$(\Delta V)v=\sum V_{out}-V_{in}$	$(c\times 10^{20})f$
(3,3)@(6,6)@(13,13)	1/2675	0/039	32/68
(4,4)@(8,8)@(14,14)	1/3142	0/034	38/35
(5,5)@(10,10)@(15,15)	1/5765	0/036	43/68
(6,6)@(12,12)@(17,17)	1/136	0/025	46/13

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