Carbon nanotube as NEMS sensor – effect of chirality and stone-wales defect intend

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Abstract. Having nanosize and unique electrical properties, carbon nanotubes (CNTs) attract lot of interest among scientific community all over the world. One of the recent observations is its role as nanosensors. Obviously the nanosize and high strength of CNT are most preferred parameter for technical and electromechanical field in the industrial point of view. The defects in CNT structure have a vital role in determining their electrical and mechanical properties. Our earlier study indicates an effective role played by the topological defects like pentagon and octagon on the electromechanical properties of these nanostructures. Here our aim is to look in to the effect of Stone-wales defect and chirality on this property of nanotubes deformed under applied pressure. Among the three kinds of tubes considered for this study, we observed that armchair (5,5) tube is more suitable for sensor applications.

1. Introduction

Carbon nanotube can be perceived as a rolled up sheet of graphite, with length up to 1 μm. Due to its unprecedented electronic and mechanical properties, it attracts both experimental and theoretical research all over the world, to explore the possibility of various technological applications like nanosensor, hydrogen storage, composites etc. The important feature of this system is their structure dependent electrical and mechanical property [1,2].

In the presence of applied stress, nanotubes get deformed and hence there is an associated change in the band gap, sometimes transferring from semiconducting to metallic type. Several researchers have thought of utilizing this property for the CNT based electromechanical sensor devices [3]. Recently it has been observed experimentally that when the middle part of suspended nanotube pushed with the AFM tip, conductivity of the tube was found to decrease depending on the tube diameter. Theoretical works related to this issue of CNT also exist [4,5]. Lin Yang and Jie Han have formulated concise form of Density of state and bandgap for deformed SWNTs from the Huckel TB model in terms of strains and chirality [6]. Alex Kleiner and Sebastian Eggert discussed deformed tube under stress [7]. They derived an analytical expression for band gaps of deformed tube including intrinsic curvature. That band gap includes deformations due to applied uniaxial stresses along the circumferential, translational directions and nanotube twist. Also they proposed that twist deformation is the only possibility to open the energy gap in armchair tube, which has no band gap in nature.

Apart from applied pressure, force etc, defects also affect the basic properties of CNTs. There are three types of defects, topological defects, rehybridization defects and incomplete bonding in carbon nanotubes. The most important topological defect “Stone-wales” defect is a combination of two pentagons and two heptagons (5-7-7-5 defect). This kind of defect causes little change to the diameter and chirality and the deformation effect is rather local. And this transformation effectively elongates the tube in the strain direction, releasing the excess strain energy. This defect is can be
incorporated in a normal tube by 90° rotation of carbon – carbon bond between two hexagons. This rotation changes four neighbouring hexagons into two pentagons and two heptagons as shown in figure 1 [8].

Figure 1. (a) (9,0) CNT  (b) (5,5) CNT with Stone Wales defect (indicated in yellow colour).

Such bond rotation defect was observed to determine the size of the band gap. For example the defects introduced in a semiconductor nanotube make the tube metallic in character by closing the band gap. The same defect in metallized CNT show much stronger one-dimensional effects than the defect-free metallic nanotube [9]. Here our interest is to discuss the effect of circumferential deformation in both metallic and semimetallic carbon nanotubes with and without Stone-wales defect under applied pressure through simulation studies.

2. Computational Details

Atom based geometry optimization have been done through Forcite module with universal forcefield. Since our model is large and to get more accurate results, we chose Conjugate gradient algorithm for this simulation. By applying external pressure, circular cross sectional tubes were compressed in to elliptical cross sectional tubes. And the radial deformation parameter \( \varepsilon = \frac{dR}{R} \) for these deformed tubes has been calculated. In recent paper it was claimed that circumferential deformation or translational deformation would affect the band gap of small band gap semiconductors [7]. We are interested in the effect of circumferential deformation on band gap energy, and it was calculated through the following expressions [7],

For Zig – zag and chiral tubes,

\[
E_g = \left[ \frac{\gamma \pi^2}{8C_h^5} + \frac{ab\sqrt{3}}{4C_h^3} \varepsilon \right] (n-m)\left(2n^2 + 5nm + m^2\right)
\]

while for Armchair tubes,

\[
E_g = \left| \frac{\gamma a^2}{16R^2} + \frac{ab\sqrt{3}}{2} \varepsilon \right| \sin 3\alpha
\]

where,

\( \gamma = 2.5 \text{ eV} \) is overlap energy
\( a = 2.49 \text{ Å} \) is lattice constant
\( b = 3.5 \text{ eV/Å} \) is the linear change in the transfer integral with a change in bond length due to deformation.
\[ C_h = \sqrt{n^2 + nm + m^2} \] where, \( n \) & \( m \) are integers

\( R \) = Radius of the tube

\( \varepsilon \) = radial deformation parameter

\( \alpha \) = chiral angle.

We have chosen achiral (9,0) semimetallic zigzag tube, (5,5) metallic armchair tube and (8,2) semimetallic chiral tube for our study. All these tubes have the same diameter of 7 Å but of different electrical properties. The details of construction of (9,0) and (5,5) symmetry tubes have been well explained by several authors while studying various issues like stress effect, adsorption etc. In order to find out the effect of chirality during applies stress, we have constructed (8,2) semimetallic tube with 68 atoms and length of the value 8 Å. We have applied external pressure from 10 GPa to 50 GPa to the considered tubes. The deformed tubes under 10 Gpa and 20 GPa are shown in Fig. 2 and 3. and it shows the elliptical deformations similar to symmetric tubes.

\[
\rho_{\Delta} = \Delta \ln 2 kT/nE_g
\]

where,

\( k \) is Boltzmann constant

\( T \) is temperature and \( \rho \) is resistivity, which is the reciprocal of conductivity (\( \sigma \)).

The bandgap variation and the conductivity values are estimated and the results are analysed in the following section.

3. Results and Discussion

Considering (9,0), (5,5) and (8,2) CNTs with and without stone-wales defect, we have calculated the bandgap energy values using Eqn. 1 and 2. The variation of bandgap with applied pressure for all the above-mentioned cases has been shown as a graph in Fig.4. Small bandgap semiconducting (9,0) tube will tear due to higher value of applied pressure. Armchair tube shows large...
variation in $E_g$, which leads to semiconducting transition and the trend agrees with existing literature [10]. While for chiral $(8,2)$ tube the results show a drastic reduction in band gap up to a stress value of at 0.8 eV.

Figures 4. Variation in bandgap of $(9,0)$, $(8,2)$ and $(5,5)$ carbon nanotubes with and without Stone-Wales defect for applied pressure.

The effect of Stone-Wales defect is observed as change in band gap, $\Delta E_g$. With these $\Delta E_g$ we have computed change in conductivity values using Eqn.3.

Table 1. Change in bandgap and conductivity for different types of carbon nanotubes under various external hydrostatic pressure

| Applied Pressure (GPa) | Change in Bandgap $\Delta E_g$ (eV) | Change in Conductivity (mho/Å) |
|------------------------|--------------------------------------|--------------------------------|
|                        | $(9,0)$ | $(5,5)$ | $(8,2)$ | $(9,0)$ | $(5,5)$ | $(8,2)$ |
| 10                     | 0.021   | 0.01    | 0.19    | 0.66    | 0.77    | 0.03    |
| 20                     | 0.03    | 0.08    | 0.03    | 0.57    | 0.21    | 0.55    |
| 30                     | -       | 0.02    | 0.10    | -       | 0.7     | 0.15    |
| 40                     | -       | 0.05    | 0.12    | -       | 0.36    | 0.10    |
| 50                     | -       | 0.04    | 0.12    | -       | 0.42    | 0.09    |

*Negative sign shows the reduction in bandgap, conductivity values.

Table 1 shows the change in band gap and conductivity corresponding to the applied pressure values form 10GPa to 50 GPa on $(9,0)$, $(5,5)$ and $(8,2)$ carbon nanotubes. Change in conductivity is linear from the value of 30 GPa. And the results show that $(5,5)$ armchair metallic tube with minimum $\Delta E_g$ finds to be a more sensitive to the applied stress and is suitable material for nanosensing application since the change in conductivity value is many fold for a particular stress value.
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