

Design and Simulation of Carbon Nanotube based Piezoresistive Pressure sensor

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Abstract: The design and performance of a piezoresistive surface micromachined circular diaphragm based pressure sensor utilizing Single walled Carbon nanotubes (SWNT) has been investigated. A structural deformation of the piezoresistive nano structure placed above the diaphragm will result in a change of resistance, which is in direct accordance with the applied pressure. This effect relies on the principle of piezoresistivity and employing a nano structure results in increased sensitivity of the sensor.

The spatial dimensions of the nanoscaled structure and its properties under investigation offer a wide range of computer modelling from force field based Molecular mechanics, Kinetic Monte Carlo, mesoscale simulation of evolving morphology, to Finite Element Method (FEM) based computation of its physical properties. The static analysis of the system under ambient temperature is performed using FEM model employing COMSOL Multiphysics. The simulated results can optimize the design parameters such as diaphragm and nanotube dimensions, for a variegated operating range of pressure and sensitivity.

Keywords: Piezoresistance, Pressure Sensor, Carbon nanotubes, FEM model.

1. Introduction

Two decades since their discovery by Iijima in 1991, Carbon Nanotubes (CNTs) have been subjected to extreme observations and detailed analysis owing to their remarkable properties [1]. This unique allotrope of carbon due to its extraordinary electronic properties and peculiar mechanical properties has received much attention in the nano-electro-mechanical systems (NEMS) community. A coalescence of interesting properties makes the carbon nanotubes as potential nanotransducers in pressure sensing applications. Modern miniaturized pressure sensors have put piezoresistive and capacitive effects into play

and a major area of concern has always been the low sensitivity of the piezoresistive materials employed. Theoretical and experimental analysis of the electromechanical properties of Single walled nanotubes (SWNT) highlights the materials' extraordinary potential and diversity.

Existing simulation models for carbon nanotubes are grounded on two fundamental frameworks namely *discrete* and *continuum* models. The discrete models provide a valuable insight in analyzing the behaviour of individual CNTs, but are restrained to small time and length scales due to immense computing power precincts. Though continuum models face a serious threat of break down in the nano regime, many assumptions and designs for modelling macro and micro mechanics are valid at nanoscale to some extent. In this design, a continuum solid model of the CNT is employed to calculate the mechanical strain experienced when it is mounted on a radial Silicon diaphragm.

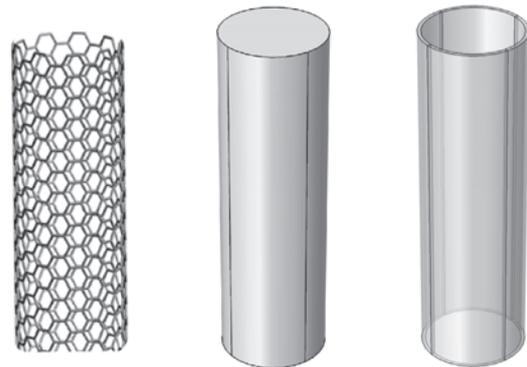


Figure 1: a) Discrete model b) Continuum Solid Model c) Continuum Shell Model

A Single-walled nanotube (SWNT) can be metallic or semi-conducting depending upon its chirality and diameter [2]. Achieving this ability without being doped opens access to a new class of solid state materials, and also an interesting issue arises as to how stretching and twisting of these carbon bonds affect the electronic

properties of the tubes. Extensive studies reveal that small gap semiconducting carbon nanotubes (SGS-CNTs) show as much as two orders of change in their electrical conductance to just about 3% strain. Dai *et al.* reported a gauge factor of 600-1000 for SGS – CNT, where as the gauge factor of silicon ranges only from 100-200[3]-[5]. The Gauge factor of a structure is the change in resistance to the amount of volumetric strain acting on it [6].

$$GF = \frac{\Delta R/R}{\varepsilon} \quad (1)$$

where R , ΔR and ε are the initial resistance of the sensor without applying pressure, resistance change of the CNT under applied pressure and the strain of the sensor, respectively.

2. Model

The pressure sensor design consists of piezoresistive CNT element resting on top of Silicon/Si₃N₄ diaphragm. A contact is established with the SWNT utilizing Platinum electrodes, thus measuring the resistance of the nanostructure. The application of pressure underneath the sensor causes a deflection of the silicon membrane and this causes a change in resistance of the Carbon nanotube. The optimal location to place the CNT would be the region of maximum strain on the diaphragm. As a result, the calculation of strain distribution and deflection in accordance with the applied pressure becomes pivotal.

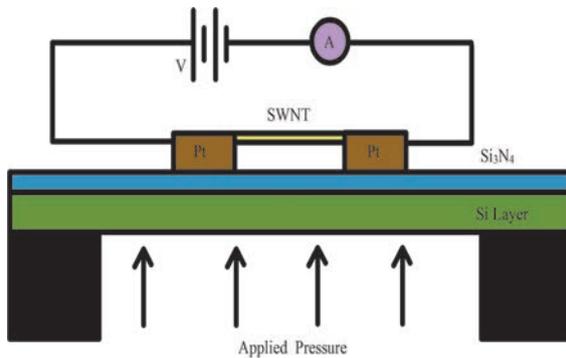


Figure 2: The Pressure sensor model

3. Mechanical Deformation analysis

The analytical solution for the maximum deformation w , caused in the circular diaphragm due to a applied Pressure P is given by (2) [6],

$$w = \frac{Pa^4}{64D} \left[1 - \left(\frac{r}{a} \right)^2 \right]^2 \quad (2)$$

where r and a are the radial coordinate and diaphragm radius, respectively. D is the flexural rigidity, and is given by,

$$D = \frac{Eh^3}{12(1-\nu^2)} \quad (3)$$

where E , h and ν are Young's modulus, diaphragm thickness, and Poisson's ratio, respectively. The difference in volumetric strain caused due to applied pressure is the major parameter of concern, as the electron conducting properties of the SWNT is strain dependent. COMSOL Multiphysics is employed to model the geometry of the pressure sensor and the deformation due to the applied pressure is found to be high at the centre.

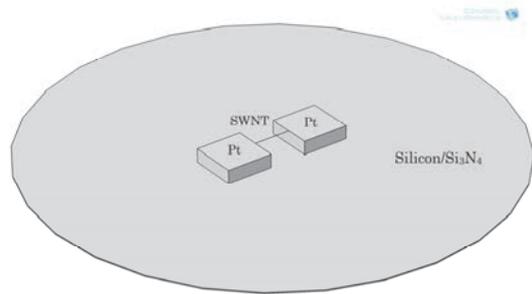


Figure 3: Pressure Sensor Geometry using COMSOL Multiphysics

Based on the theoretical deformation found using the FEM model, the CNT's change in its molecular structure and the strain induced change in its resistance can be modeled. The high aspect ratio of the Carbon nanotube and its size significance when compared to that of the diaphragm dimensions plays a major role in applying the mesh formulation of the pressure sensor. The diaphragm of 1 μm thickness (Si/Si₃N₄) and 250 μm radius is modeled and the deformation is theoretically obtained for a pressure range of 1 kPa to 500 kPa. The maximum volumetric strain acting on the SWNT

($d \sim 5\text{nm}$) is obtained using Solid mechanics module in COMSOL Multiphysics. The results are plotted in Figure 7.

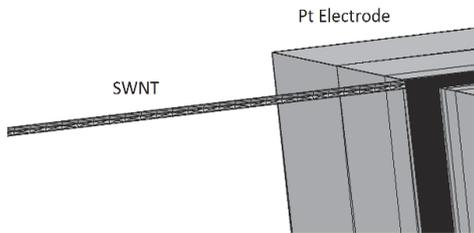


Figure 4: Mesh of the contact region between Single Walled Carbon Nanotube and Platinum electrode

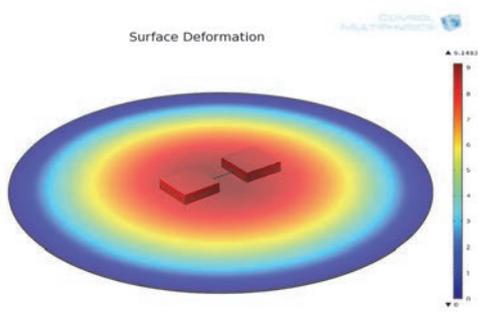


Figure 5: Surface deformation of the CNT based pressure sensor for 150 kPa pressure

The other parameters that affect the volumetric strain of the SWNT include the membrane thickness, the membrane size and the release height of the SWNT from the membrane. A SWNT sited at a release height of $14.995\ \mu\text{m}$ from the membrane, when subjected to a 150 kPa pressure on the diaphragm experiences a volumetric strain of 1.02% as shown in figure 6.

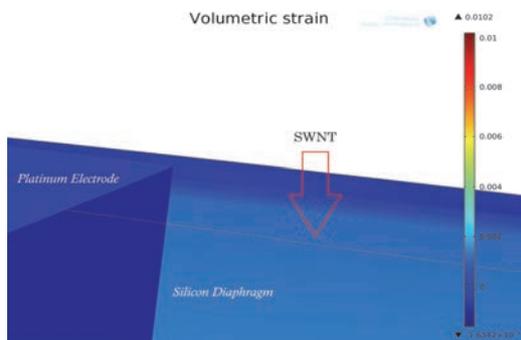


Figure 6: Volumetric strain on SWNT under an applied Pressure of 150 kPa on diaphragm

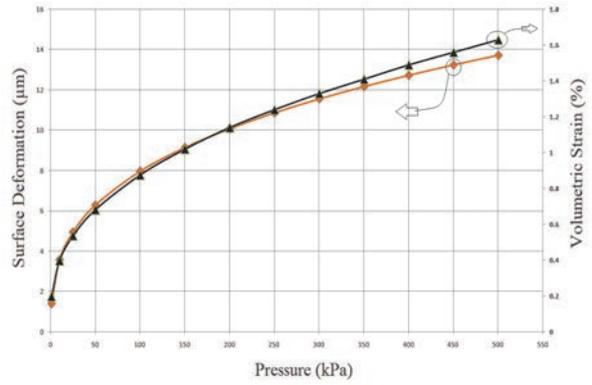


Figure 7: COMSOL simulation results i) Surface Deformation and ii) Volumetric strain vs. Pressure

4. Piezoresistance of CNT

The Volumetric strain of the carbon nanotube obtained from the FEM analysis of COMSOL Multiphysics is utilized to compute the strain dependent band gap and thus the resistance of carbon nanotubes is obtained. Previous studies on the band gap of SWNT have revealed its dependence on strain. The strain- dependent band gap of an ideal ballistic SWNT is expressed by [6]-[11],

$$E_g = E_g^0 + \frac{dE_g}{d\varepsilon} \varepsilon \quad (4)$$

where,

$$E_g^0 = |p|2\gamma a_0 / (\sqrt{3}d) \quad (5)$$

and

$$\frac{dE_g}{d\varepsilon} = \text{sign}(2p+1)3\gamma[(1+\nu) \cos 3\theta_l] \quad (6)$$

where γ is the tight-binding overlap integral or the hopping integral ($\sim 2.6\ \text{eV}$), $a_0 \sim 2.49\text{\AA}$ is the graphene lattice unit vector length, d is the diameter of the SWNT, θ_l is its chiral angle, and $p = 0, \pm 1$ labels the nanotube family. The family index p is given by the chiral index (n, m) in terms of determining p from $n-m=3q+p$, where q is an integer and p is $-1, 0,$ or $+1$. The change in band gap energy with respect to strain ($dE_g/d\varepsilon$) is < 0 for families of semiconducting tubes $p = -1$ and > 0 for $p = +1$. The strain dependent band gap energy of the semiconducting SWNT is computed based on equations (4), (5) and (6).

The resistance of a carbon nanotube depends on its energy band gap and is given as [9],

$$R_{tot}(\epsilon) = R_s + \frac{1}{|t|^2} \frac{h}{8e^2} \left[1 + \exp\left(\frac{E_g}{kT}\right) \right] \quad (7)$$

where R_s is the contact resistance in series, $|t|^2$ is the transmission coefficient, h is the Planck's constant, e is the electron charge, k the Boltzmann's constant, T is the absolute Temperature and E_g is the strain dependent band gap energy. The resistance R_{tot} at zero strain is utilized to find the gauge factor of the CNT sensor as given by (1). Since the design has a metal on tube end contact to measure the resistance changes due to strain, the contact resistance R_s of the CNT with the platinum electrode is assumed to be 50 k Ω [12],[13]. The other parameters of the CNT considered for obtaining the gauge factors are tabulated below.

Chiral index (n, m)	(49, 24)	(50, 24)
Diameter (d nm)	5.048	5.122
Chiral angle (θ deg)	18.81	18.53
p ($3q+p = (n-m)$)	+1	-1
$ t $ (transmission probability)	0.5	0.5

Table 1: Parameters of SWNT

Now the volumetric strain obtained from the COMSOL FEM model is utilized in (4) and the result is fit in (7) to obtain resistance value of the SWNT in the high strain regime.

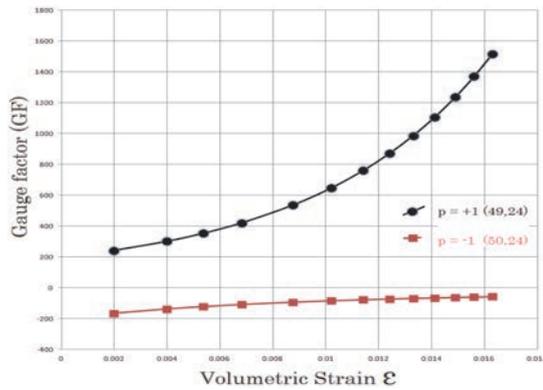


Figure 8: Gauge factor vs. Volumetric Strain

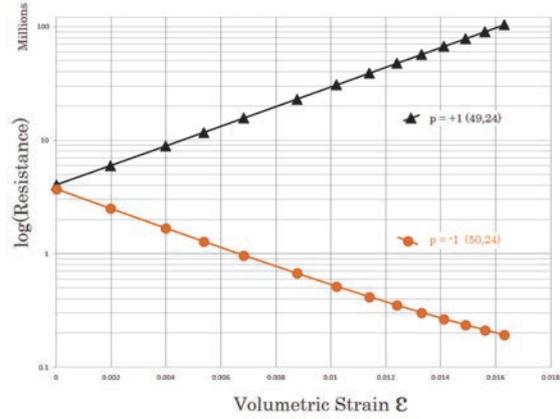


Figure 9: $\log(\text{Resistance})$ vs. Volumetric Strain ($p=+1$ and -1)

The change in resistance due to the applied strain and Gauge factors for both the families of CNTs ($p = \pm 1$) are calculated and the results are shown in figures 8 and 9. The positive piezoresistive gauge factor ($p=+1$) is found to reach around 1500 which is extremely sensitive than the state of the art silicon technology (~200). The sensitivity of the pressure sensor is given by,

$$S = \Delta R / \Delta P \quad (8)$$

where ΔR is the change in resistance and ΔP is the change in pressure. A plot of Sensitivity against pressure is depicted in Figure 10.

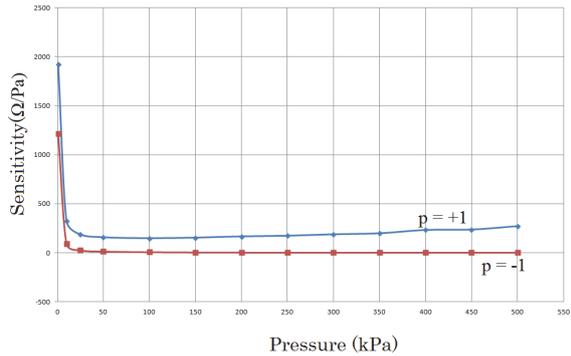


Figure 10: Sensitivity vs. Pressure

Thus as a result of the sensitivity plot it is clear that the positive semiconducting family is found to be more sensitive than the negative semiconducting family.

5. Conclusions

The modeling of a CNT based piezoresistive pressure sensor using COMSOL Multiphysics has been discussed. Theoretical simulations show the gauge factors obtained for a single walled nanotube of particular chiral dimension. Optimizing the design for better gauge factors and sensitivity can be done through the simulated model. However, the chiral indices of the investigated SWNT and the contact resistance R_c cannot be precisely fabricated until advanced techniques emerge for both manufacturing process of CNT and its manipulation. The simulation shows that different chiral indices of CNTs are useful to obtain different gauge factors and sensitivities. Moreover the piezoresistive gauge factors of current day pressure sensors in use are totally shadowed by the promise rendered by these beautiful tubes of carbons.

6. References

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