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# Sensitivity analysis of nems cantilever to detect volatile organic compounds using finite element method

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## Abstract

Nano Electro Mechanical System (NEMS) based cantilever is the alternate form of Micro Electro Mechanical system (MEMS) with dimensional changes in perspectives like thickness, length, and width. The advantage of the dimensional change leads to great improvement in sensitivity and performance with portable structure. In this paper, a stepped nanocantilever sensor is designed for the detection of volatile organic compounds. The same is compared with the conventional micro cantilever in order to assess the sensitivity. The advantage of incorporating longitudinal cut at fixed end of the cantilever is investigated for different materials with load analysis and stress distributed results. COMSOL Simulation software is used to perform the analysis of nanocantilever and the result shows sensitivity increased with longitudinal cut and type of material which exhibits good sensitivity. In this research, we suggest a stepped cantilever structure that uses FEM to calculate the change in deflection owing to various loads in both static and dynamic analyses. Similarly, changes in resonance frequency for changes in beam thickness are examined using parametric study. The experimental results from COMSOL simulation are found that the displacement occurred in proposed cantilever that the deflection sensitivity 2.85 x$10^{-9}$m under maximum stress of 3.32 x$10^{-9}$ N/$m^2$. From the dynamic analysis, resonant frequency occurs at 20nm thickness is 2.8x$10^{7}$ Hz, and at 30nm is 3.5 x $10^7$ Hz respectively.

**Keywords:** Cantilever; Gas detection; MEMS; NEMS; VOC.

## 1. Introduction

VOCs are any of the thousands of organic compounds that exist mostly as gases at normal temperature (Pandey and Yadav, 2018). Carbon monoxide is not included in the above definitions of inorganic carbon since it comprises gases such as carbon oxide. VOCs are chemical substances that may be man-made or natural gases. VOCs are a diverse group of chemicals that may be employed in a number of ways, depending on the kind of chemical bonds and the structure of the compounds. Some chemicals that may be employed in MEMS applications include acetone, benzene, and ethanol (Gębicki, Dymerski & Namieśnik, 2017 and Schütze *et al.*, 2017). There are several causes that contribute to the presence of gases in the environment. Tobacco smoking, construction materials, consumable items, and chemical processes are examples (Szulczyński &

Gębicki, 2017).However, VOCs are suspected of causing a number of health consequences that happened during chemical oxidant and adjacent locations. Overall, the biggest concern with voc is the health repercussions of various chemical reactions (Leidinger *et al.*, 2014).

Because of the advancements in technology now a day's miniaturized devices are feasible with micro machining processes (Katta & Lavanya, 2021). They have benefits like portability, economical, energy efficient and more responsive. They also provides advantages like, accommodate most complex electronic circuitry in a small die area with high performance features(Miranji Katta & Sandanalakshmi R, 2020). By understanding the key features of Nanotechnology NEMS based cantilever are gaining advantage over MEMS in the all domains. More over Nano scale devices are easier to interact with gas molecule on both surface and inside the cells. Conventional sensing system requires complex electronic interfacing with packaging and maintenance. All these limitations are avoided by using NEMS based cantilever is used as gas detector(Neethu & Suja, 2016 and Blaikie, Miller & Alemán, 2019) . When surface cantilever undergoes chemical or physical reaction based on organic compounds (Prakash & Siddaiah, 2021).

In the process of detection, imparting specimen sample at the free end surface area of cantilever structure, it undergoes displacement and vibrations. Then analyze relative shift in resonance frequency due to change in vibration or displacement can predict the mass of specimen sample located at sensitive end of the NEMS cantilever(Siddaiah *et al.*, 2019). So as to observe the external signal it is mandatory to interpret resonance frequency or displacement due to mechanical and electrical equivalent characters(Srinivasa Rao Karumuri, 2016 and Siddaiah & Manjusree, 2017).

## 1.1 Background

Existing commercially available VOC detectors operate on the principles of photoionization detectors (PID), electro-chemical sensors, metal-oxide- sensors (MOS)(Khaleel & Hashim, 2020), optical sensors, portable or micro gas chromatographs (MGC), and flame ionization detectors (FID)(Kalambe & Patrikar, 2014). As a result, a microcantilever is a device that can perform chemical, physical, or biological sensors to detect changes in cantilever bending. On a flat object, a cantilever's deflection causes a change in mass of analyte, which is precisely retained (Szulczyński & Gębicki, 2017). Micro cantilevers are already a million times smaller in microns. Deflection of a microcantilever sensor is caused by molecules absorbed on it (Siddaiah & Manjusree, 2017). Piezoresistive deflection, optical deflection, capacitive deflection, optical diffraction grating, and charge coupled device are all investigated for deflection detection (Katta *et al.*, 2019 and Rahul & Kumar, 2019).

The VoCs are very small in size in the order of nanometer. The detection of such smallest VoCs requires sensors which are capable to provide high sensitivity with specificity and good selectivity(Katta & Lavanya, 2021). To meet these requirements NEMS based cantilever structure is more suitable in order to detect VoCs. NEMS cantilever structure provide satisfied result in the detection of VoCs because of their quantum sensitive range of geometrical structure(Siddaiah *et al.*, 2019). Here cantilever structure uses the principle of Mechanical and electrical transduction mechanism. If the stress created on free end of the cantilever owing to adsorption of gas molecule as shown in below Figure 1.

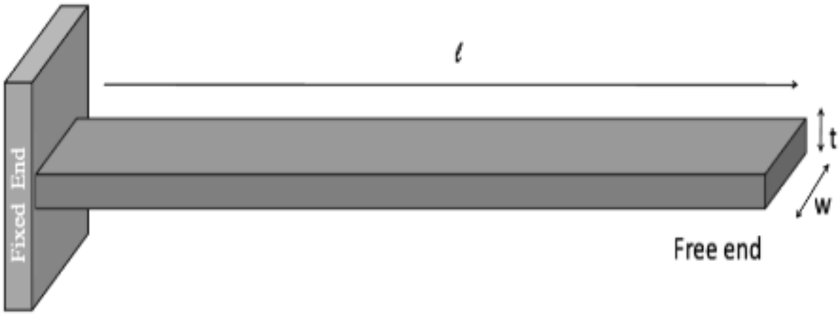


**Fig. 1.** Conventional cantilever beam

Here the deflection of beam due to binding of targeted molecules with an analytes on the high sensitive surface leads to change in resistance(Siddaiah & Vamsi Aravind Swamy, 2019) . This change in resistance occurred in cantilever structure is easily measured with a micro ammeter or voltmeter.

## 2. Design methodology:

The mounting structure of the cantilever beam has one fixed end and one free end just like a spring–mass system(Wieczorek & Jeleń, 2019). The important parameters of cantilever beam which makes it suitable for desired applications are resonant frequency and deflection sensitivity under static and dynamic modes(Miranji Katta & Sandanalakshmi R, 2018). These two parameters depends on the material characteristics like Poisson's ratio, young's modulus, and geometrical parameters such as length, width and thickness of a cantilever beam.

To analyze the geometrical characteristics of basic cantilever structure, consider the general force balance equation of spring-mass system(Katta *et al.*, 2020).

$$F_x = m\frac{d^2\mathrm{y}}{\mathrm{d}t^2} + \gamma\frac{\mathrm{dy}}{\mathrm{dt}} + k(y - y_0) \tag{1}$$

Where m is the mass of cantilever beam $\gamma$ is the damping factor, y and $y_0$ are change in deflection before and after mass is applied, F is the external force, k is the spring constant depends on material properties.

$$k = \frac{3EI}{l^3} \tag{2}$$

E is the young's modulus of the material in Pa, I is the moment of inertia, length of the beam in meters. The cantilever beam equivalent of the same mass which allowed by spring mass system is numerically equivalent to

$$m_b = \eta_1 \rho_b \, lwt \tag{3}$$

$$k_b = \frac{\eta_2 E_b I_b}{l^3} \tag{4}$$

$$I_b = \frac{wt^3}{12} \tag{5}$$

Where subscript **b** indicates the before Gas molecule placed on its surface, $\eta_1 \& \eta_2$ are the constant, depends on how fixed end the cantilever beam suspended, $\boldsymbol{\rho_b}$is the density of the cantilever**, l, w, t** are the length, width and thickness respectively. The spring coefficient **k** changed with mass, hence above equation (3), (4) and (5) before mass is applied.

## 2.1 Effect of mass on resonant frequency:

In this paper simple double layer cantilever proposed with and without longitudinal cut at fixed end. Assume that the Gas molecule is landed on the surface of the cantilever beam, then the equations (3),(4),(5) becomes

$$m_a = \eta \rho_a \, lw(t + \Delta t) \tag{6}$$

$$k_a = \frac{3E_a I_a}{l^3} \tag{7}$$

$$I_a = \frac{w(t + \Delta t)^3}{12} \tag{8}$$

Here subscript **a** indicates after Gas molecule is placed on the surface beam. Now consider the ideal case, assumed to be as no damping and continuous external force but a little push to the cantilever to observe how the mass related with natural frequency, from the equation (1)

$$m \frac{d^2(y_0 + \Delta y)}{\mathrm{d}t^2} + k\Delta y = 0 \tag{9}$$

Where $y_0$ is constant, and obtain the solution for above equation, we get

$$\Delta y = \alpha e^{J\omega_0 t} \tag{10}$$

$$\omega_0 = \sqrt{\frac{k}{m}} \tag{11}$$

Where $\omega_0$is the natural frequency of the cantilever beam. If Gas molecule are landed before and after, on the surface of the cantilever beam, resonance frequency from equation (11) becomes

$$\omega_{ob} = \sqrt{\frac{k_b}{m_b}} \tag{12}$$

$$\omega_{oa} = \sqrt{\frac{k_a}{m_a}} \tag{13}$$

While substituting the terms from equation (3) and (4), (6) and (7) in above (12) and (13) gets resonance frequency of the cantilever beam in two cases.

When molecule landed cantilever surface then change in mass, spring coefficient

$$m_a = m_b + \Delta m \tag{14}$$

$$k_a = k_b + \Delta k \tag{15}$$

While substitute equation (14) and (15) in equation (13) to obtain net change in resonant frequency due to added mass.

$$\frac{\Delta\omega}{\omega_b} = \frac{\Delta k}{2k_b} - \frac{\Delta m}{2m_b} \tag{16}$$

Assume spring coefficient k is negligible and simplify above expression using equation (3),(4), (5) we get

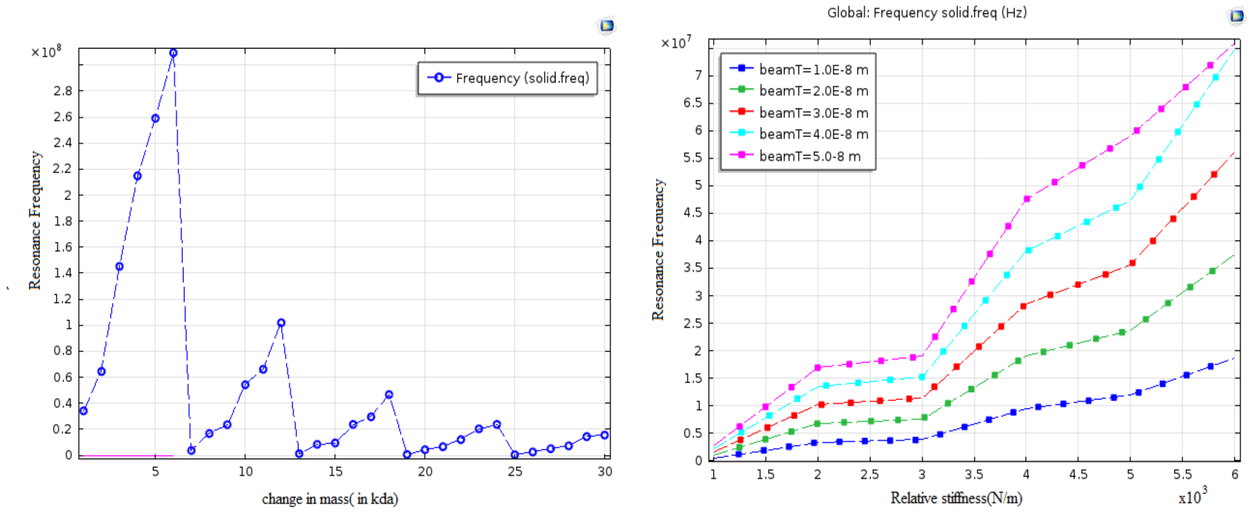
$$\Delta\omega = -\frac{\Delta m}{2}\sqrt{\frac{\eta_2 E_a}{12\rho_a^3\eta_1^3}\frac{1}{wl^3}} \tag{17}$$

From the above equation (17), it is observed that net change in frequency directly proportional to mass landed on the cantilever surface $\Delta m$ and inversely proportional to geometrical characteristics of cantilever beam such as width and length $w, l^3$. it also depends on properties of material which is used to fabricate the cantilever. Figure 2(a) shows simulation response of change in resonance frequency with respect to mass.

2.2 Effect of Stiffness on resonant frequency:

In the previous case only mass is considered, and spring coefficient is omitted. When multiple layers are coated on the cantilever surface its stiffness becomes considerable factor in cantilever sensitivity. To obtain the expression for stiffens of the beam, assume Gas molecule mass is negligible from the equation (16), and substitute equation (3), (4), (5) and simply

$$\Delta\omega = \frac{\Delta k}{2}\sqrt{\frac{12\eta_1\,\rho_b\,l^4}{\eta_2\,E_b\,wt^2}} \tag{18}$$



(a) (b)

**Fig. 2.** Parametric sweep results (a) Change in Resonance frequency with respect to VoCs Mass (b) Relative stiffness of cantilever beam Versus Resonance Frequency

From the equation (4) and (5), $\Delta k$ is strongly depends on thickness of the cantilever beam $(\Delta t)$, the thickness of the beam again varied with respect to dimensions of the Gas molecule may be no. of molecules, area of each molecule and its thickness, other coatings if any. From the equation (18), resonant frequency of the cantilever beam is proportional to change in stiffness or spring coefficient of the beam, figure 2(b) shows the simulation results of change in resonant frequency with respect to stiffness. In the nano scale range, equation (18) shows the significant effect when modulation of **k** due to molecular capture on cantilever typically 10 – 40% change.

## 2.3 Static deflection:

In the previous section we discussed about factors involved in dynamic biosensing, but it not work alone in detection of small particles. Hence static deflection of beam is also considered in nano scale structure. Under the static deflection measurement, from the equation (1) time varying components becomes zero i.e.

$$ky = \; F = mg \tag{20}$$

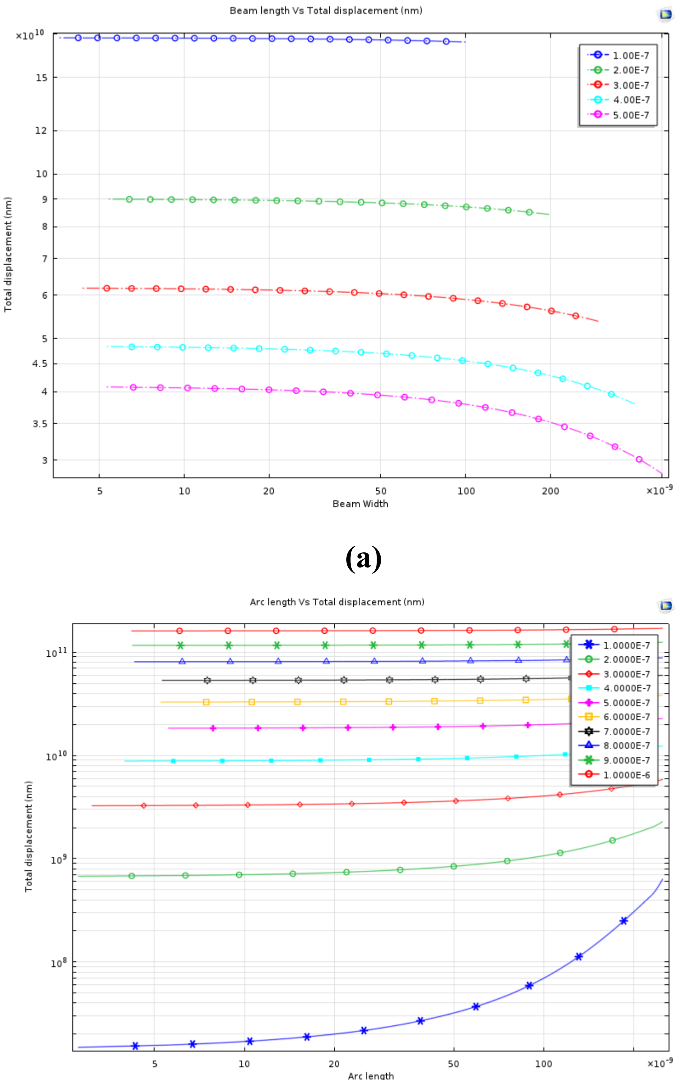
By simplified and apply logarithm, differentiation on both sides with respect to its real values we get

$$\frac{\Delta y}{y_o} = \frac{\Delta m}{m_o} - \frac{\Delta k}{k_o} \tag{21}$$

For an instance consider a mass induced deflection on silicon fabricated cantilever beam with length-250nm, width-75nm, thicknes-20nm, Density ($\rho_{si}$) - 2330kg/m$^3$, pathogenic elements with dimensions length-250nm, width-75nm, thickness-40nm, Density ($\rho_p$) – 1220kg/m.

From the equation (21), with a negligible spring coefficient gives great deflection sensitivity, but it is impractical. When we consider the basic equation (20), get the deflection of 41.07fempto meters (fm). This is practically immeasurable. To address this problem if somehow improve the spring coefficient k gives better measurable deflection

## 2.4 Effect of length on deflection sensitivity:



**(a)**

**(b)**

**Fig. 3.** Change in deflection sensitivity (a) Change in total deflection with respect to beam width (b) Change in Deflection with respect to arc length.

### 2.5 Stoney's formulation with respect to geometrical structure:

According to the stoney's equation, the relation between deflection sensitivity and stress on a rectangular cantilever beam

$$ds = \frac{4(1-v)\sigma L^2}{Et^2} \tag{22}$$

Where d**s** is the deflection sensitivity and $\boldsymbol{v}$is the Poisson's ratio, **L** is the length of cantilever beam, **E** is the young's modulus and **t** is the thickness of the beam, **σ** is the stress applied on the surface.

Similarly the electrical behavior of resonant frequency of cantilever structure in its mechanical equivalent as spring constant **k**, related by

$$k = \frac{E\omega t^3}{4L^3} \tag{23}$$

Where $\omega$ is the vibrational as resonant frequency

According to the above stoney's equation (Katta *et al.*, 2020) deflection of cantilever beam is proportional to stress applied on its surface under the assumption of small and fixed geometrical parameters length and thickness.

The resonant frequency of the cantilever beam with mass density ρ is related as

$$f = \frac{\sqrt{E}t}{2\pi\sqrt{\rho}L^2} \tag{24}$$

From the above equation, it is observed that cantilever thickness is proportional to resonant frequency but length becomes inverse relation meanwhile, from the equation (1) deflection of the beam increase with length. Therefore the sensitivity of cantilever beam by considering deflection and frequency i.e. from equation (1) and (3) defined as

$$ds * f = \frac{2(1-v)\Delta\sigma}{\pi\sqrt{E\rho}t} \tag{25}$$

The cantilever stiffness coefficient **k** also plays a key role in determining factor of sensitivity along with characteristics of a material and geometrical structure. From this analysis it is observed that sensitivity of a cantilever beam varied with respect to shape and type of the material used to design cantilever beam. This concept is explained by Hooke's law as F = -KX where Negative symbol indicates restoring force. Figure 3(a) & (b) shows net change in displacement with respect to beam width and length respectively.

## 3. Materials and methods:

Before going to design nems based cantilever beam, it is necessary to check whether which material possess good deflection sensitivity. So this section will cover different silicon based materials, and structural cantilever is designed and simulated using COMSOL simulation software.

**Table 1.** List of materials and their properties

| Material | Youngs Modulus ($10^{11}N/m^2$) | Poisson's Ratio ($g/cm^3$) | Denity($g/cm^3$) |
|---|---|---|---|
| $SiO_2$ | 0.73 | 0.15 | 2.27 |
| SiC | 0.74 | 0.45 | 3.21 |
| $SiN_4$ | 2.50 | 0.23 | 3.10 |
| $Al_2O_3$ | 2.15 | 0.33 | 3.98 |

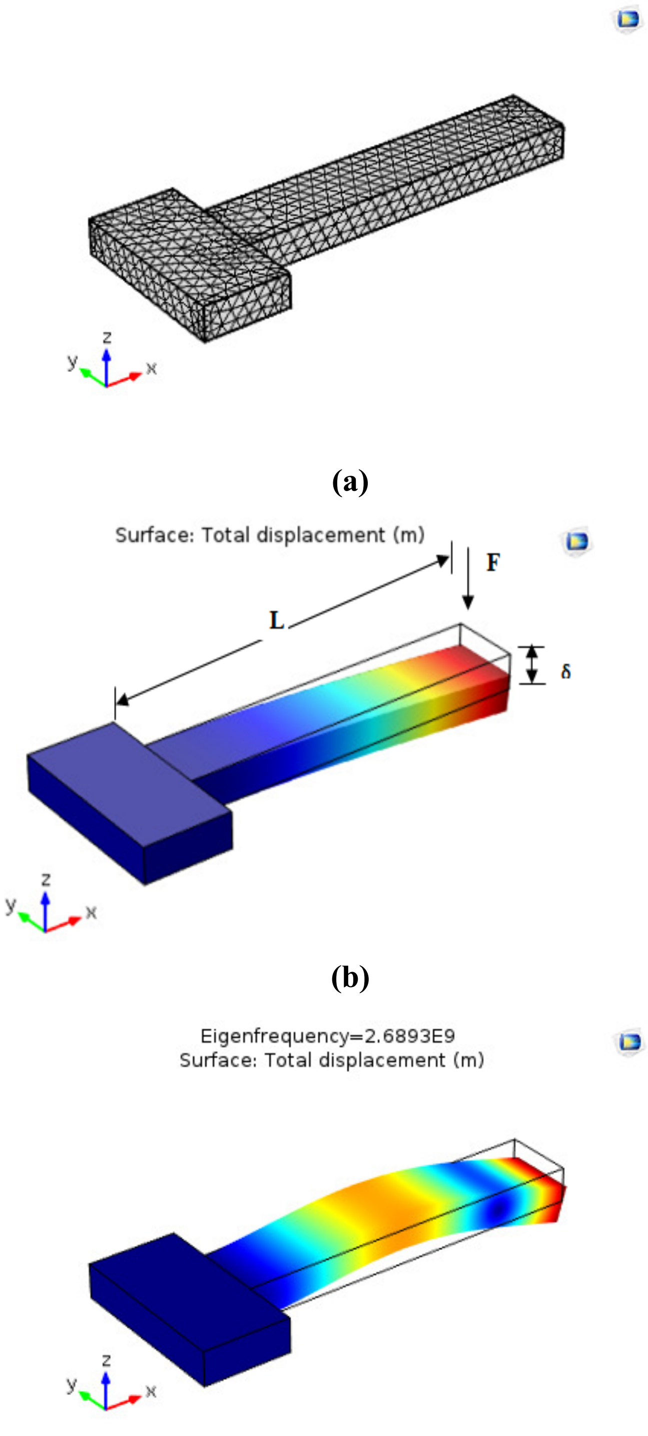
The deflection sensitivity and resonant frequency of any material depends on their geometrical structure and material characteristics like young's modulus, Poisson ratio, elasticity the same is shown in Table 1 Figure 4 shows the deflection of single layer cantilever beam over different materials for fixed load of 1nN.

Sensitivity of a cantilever beam is varied with respect to its geometrical dimensions. Form the equations (1) and (2) it is evident that deflection sensitivity is increased with length for fixed breadth and thickness vice versa. Figure 2 and Figure 3 shows that deflection sensitivity of a cantilever beam for different materials has a fixed width and thickness with variable length. From the numerical analysis of above said materials silicon and its compounds based cantilevers has reduction in resonant frequency is insignificant compared to other polymer cantilevers(Katta *et al.*, 2019 and Finot, Passian & Thundat, 2008). The silicon material has excellent thermal and mechanical properties with high elasticity it will not affected by external excitations( Zhou *et al.*, 2009 and Blaikie, Miller & Alemán, 2019).

### 3.1 Geometry dynamic analysis

To perform the qualitative analysis on cantilever beam, we must consider the their basic principle i.e. due to the presence of external force or load on surface of the beam leads to measurable deflection in static mode (Srinivasa Rao Karumuri, 2016 and Priyadarsini, Das & Dastidar, 2016), are noticeable change in resonant frequency in dynamic mode. Load imposed on surface of the beam may ranges from few nanograms to several grams depends on its geometrical characteristics and fabricated material (Siddaiah & Manjusree, 2017 and Krishna *et al.*, 2011).

To analyse the behaviour of MEMS or NEMS cantilever, we have to understand the two essential equation (22). In that first one is the Stoney's equation, which gives the relation between induced deflections due to surface stress with respect to material properties and geometrical parameters of the cantilever beam.



**(a)**

**(b)**

**(c)**

**Fig. 4**. Single ended cantilever designs (a) FEM Analysis (b) Deflection of a beam (c) Resonant frequency of a beam

## 4. Results and discussions:

Among the above said materials, most commonly used semiconductor materials are Silicon(Si), silicon dioxide($SiO_2$), poly silicon, silicon carbide(SiC) and silicon Nitride($SiN_3$). These materials are thermally strong enough and chemically more viable. In this paper, we proposed double layer cantilever structure with longitudinal cut near fixed end with enlarged rectangular free end to provide bimolecular interactions at the surface. Which exhibits relatively good sensitivity compared to conventional cantilever beam is analyzed using COMSOL simulator.

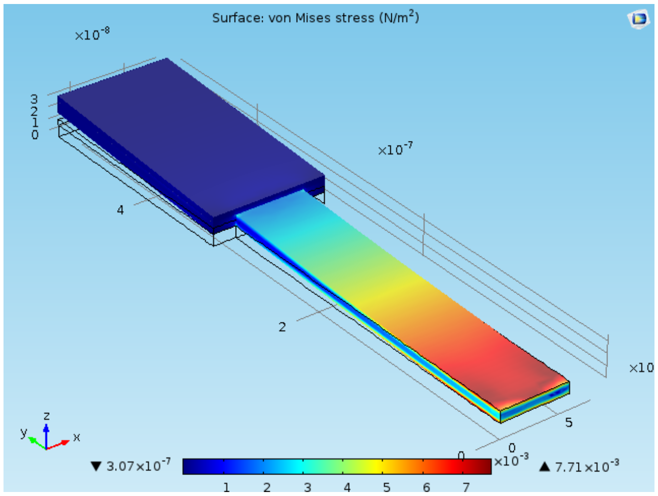


**Fig. 5.** Proposed stepped NEMS cantilever

Above Figure 5 shows conventional double layer cantilever, except the base layer, top layer is the super conductive material is used to exhibits very low resistivity and accommodate suitable environment for bimolecular interactions with chemical sensing. Table 2 shows deflection sensitivity of double layer cantilever for three different materials with variable load imposed on its free end surface. Figure 5 gives the graphical presentation of deflection sensitivity versus load. Which shows the same double layer cantilever but providing longitudinal cut at the fixed end provides relatively very good sensitivity compared to conventional cantilever structure.

**Table 2.** Load versus deflection of NEMS cantilever

| Load in nN | Deflection in nm | | |
|---|---|---|---|
| | SiC+Au | Si2N3+Au | $Al_2O_3$+Au |
| 50 | 0.7046e-11 | 2.2926e-11 | 1.4371e-11 |
| 100 | 1.4919e-11 | 4.5851e-11 | 2.8743e-11 |
| 200 | 2.9838e-11 | 9.1702e-11 | 5.7485e-11 |
| 300 | 4.4758e-11 | 1.3755e-10 | 8.6228e-11 |
| 400 | 5.9677e-11 | 1.8340e-10 | 1.1497e-10 |
| 500 | 7.4596e-11 | 2.2926e-10 | 1.4371e-10 |
| 1000 | 1.4919e-10 | 4.5851e-10 | 2.8743e-10 |

Table shows deflection sensitivity of cantilever beam with longitudinal cut for three different materials with variable load. In comparison with conventional double layer cantilever it provides high deflection for the same load.

**Table 3**. Load versus deflection

| **Load in nN** | **Deflection in nm** | | |
|---|---|---|---|
| | **Sic-N** | **$Si_2N_3$-N** | **$Al_2O_3$-N** |
| 50 | 1.1157e-11 | 3.3614e-11 | 2.1045e-11 |
| 100 | 2.2316e-11 | 6.7228e-11 | 4.2091e-11 |
| 200 | 4.4631e-11 | 1.3446e-10 | 8.4182e-11 |
| 300 | 6.6947e-11 | 2.0168e-10 | 1.2627e-10 |
| 400 | 8.9262e-11 | 2.6891e-10 | 1.6836e-10 |
| 500 | 1.1158e-10 | 3.3614e-10 | 2.1045e-10 |
| 1000 | 2.2316e-10 | 6.7228e-10 | 4.2091e-10 |

Figure 6 shows plot between deflection sensitivity over Load of cantilever beam with longitudinal cut. The NEMS cantilever beam with longitudinal cut at stress concentrated region shows good deflection sensitivity. The longitudinal cut at the fixed end used as stress concentrated region here. The dimensions of this cantilever structure is taken as overall length 750nm, width 20nm, thickness of base layer 10nm, gold coating at the surface layer 5nm

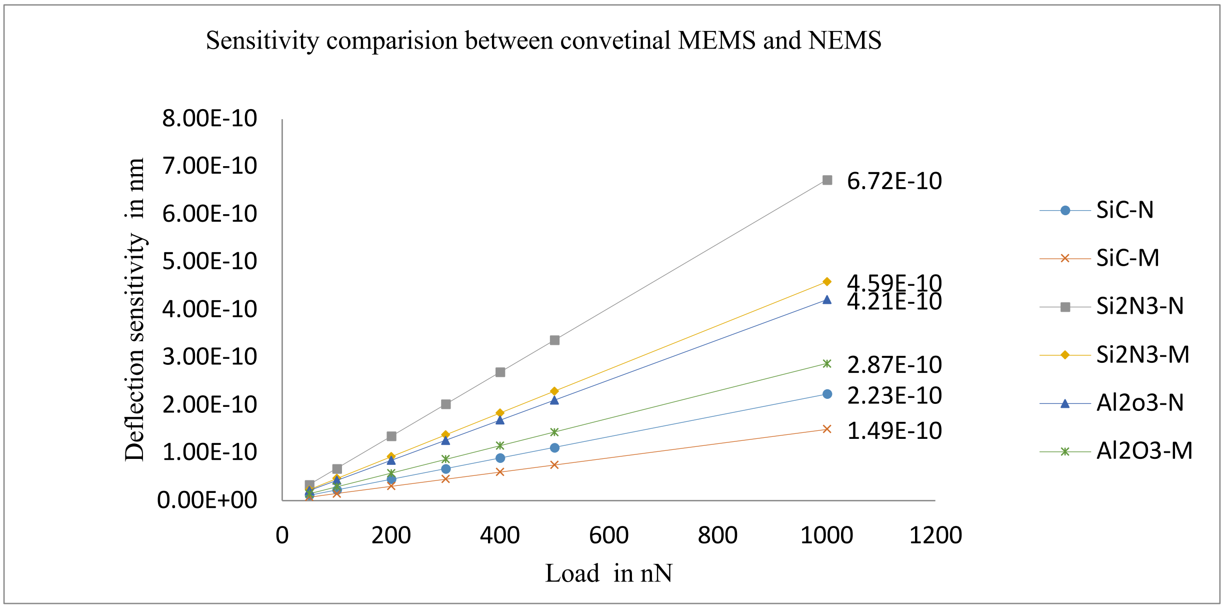


**Fig. 6.** Comparison between double layer cantilever beam sensitivity with and without longitudinal cuts

The significant effect of longitudinal cut near fixed end is analyzed using misses stress value on the beam. From the figure 4 and 6 Misses stress is calculated to find yielding condition of beam under the load. It gives the maximum operating capability of the material without fail beyond its strength. By analyzing the structure of double layer cantilever beam with and without longitudinal cuts at stress concentrated regions, from the Figure 6, longitudinal cut incorporated cantilever beam shows good deflection sensitivity. Among the three different materials for a given dimensions Silicon nitride with a gold coated surface shows good sensitivity.

## Conclusion:

The high sensitive NEMS cantilever is designed to detect the organic compounds available in closed environments. In order to develop a VOCs detection sensor this paper provides a preliminary solution to improve the sensitivity. From the above analysis sensitivity of sensor can be improved by varying geometrical dimensions such as length, width and thickness. The sensitivity of a cantilever beam increased with its length and decreased with thickness. Certainly several coatings on base layer of cantilever surface may increase the thickness. Similarly, the significant changes in resonance frequency for changes in beam thickness are examined using parametric study. The experimental results from COMSOL simulation are found that the displacement occurred in proposed cantilever that the deflection sensitivity 2.85 $x10^{-9}$m under maximum stress of 3.32 $x10^{-9}$ N/$m^2$. From the dynamic analysis, resonant frequency occurs at 20nm thickness is 2.8$x10^7$ Hz, and at 30nm is 3.5 x $10^7$ Hz respectively.

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