# Carbon Nanotube-based Ultra-sensitive Breath Acetone Sensor for Non-invasive Diabetes Diagnosis

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## Abstract

In this project, the design and theoretical analysis of an ultra-high sensitive breath acetone sensor based on carbon nanotube (CNT) structure is proposed. In this device, a carbon nanotube is anchored to a substrate in one end, and the other end is coated by ε-$WO_3$. As a ferroelectric material, ε-$WO_3$ has high selectivity in acetone absorption. The end tip of carbon nanotube is coated with ε-$WO_3$ material to absorb minute acetone molecules in breath sample. Piezoelectric activation is used to activate the vibration of carbon nanotube cantilever structure. When acetone molecules are absorbed by the coated ε-$WO_3$, the resonant frequency of the cantilever will be changed for a certain amount. By sensing this certain resonant frequency change, the existence of a single acetone molecule can be detected. A theoretical model is developed to describe the vibration of the carbon nanotube cantilever structure. The resonant frequency change of the cantilever due to attached mass is analyzed. The proposed breath acetone sensor can achieve extremely high sensitivity in molecular level. It can be potentially used for non-invasive diabetic's diagnosis, which leads to a quick, convenient, accurate and painless breath diagnosis of diabetics.

## Introduction

Carbon Nanotubes (CNTs) are molecular-scale tubes of carbon with hollow cylindrical molecular structure. Due to their unique hollow tube molecular structure, CNTs have many outstanding properties. They are the stiffest and strongest fibers known, they can be metallic or semiconductor depending on their chiralities, and have extremely large surface-to-volume ratio. CNTs can be used in many applications such as medicine, electronics, optics, architectural and other fields of material science.

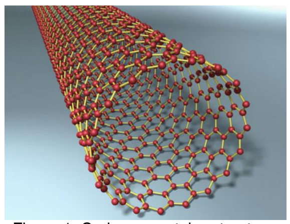

Figure 1. Carbon nanotube structure

Diabetes is a serious threat to human health. Traditional blood test for diabetes diagnosis is painful, and may lead to cross infection of blood-transmitted diseases. Non-invasive diabetes diagnosis is in a pressing need. It is known that diabetic patients have minute acetone in their breath, which can be used for diabetes diagnosis. Such minute acetone is difficult to be sensed by traditional sensors. In this project, we are developing an ultra-high sensitive acetone sensor based on carbon nanotube structure, which can be used for breath diagnosis of diabetes.

## Device Design and Analysis

The sensing of acetone molecule is achieved by measuring resonant frequency change of carbon nanotube cantilever structure before and after absorbing acetone molecules. As shown in Fig. 2, a carbon nanotube is anchored to substrate in one end, and the other end is coated by ε-$WO_3$. As ferroelectric material, ε-$WO_3$ has high selectivity in acetone absorption. Carbon nanotube is activated by piezoelectric actuator to vibrate. Its resonant frequency depends on the mass distribution of CNT. If acetone molecules from breath sample are absorbed to CNT, its mass will change, hence the resonant frequency is changed. By measuring this frequency shift, we can detect the existence of even one single acetone molecule in the breath sample.

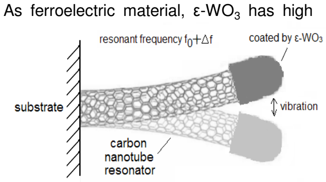


Figure 2. CNT based acetone sensor

The complete diabetes breath test system is shown in Fig. 3. A CNT cantilever array is sealed inside a tube with one end connected to a gas flow meter, and the other side connected to a sampling bag. The breath sample of a patient is input to the gas flow meter to measure its mass flow rate. It then passes through the tube with carbon nanotube sensor array. A sampling bag is used to collect the breath sample after absorption for further analysis. A monitor is anchored on the surface to display result.

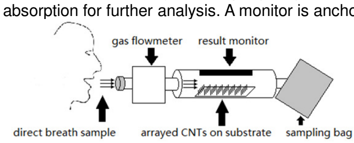


Figure 3. CNT based diabetes breath analysis system

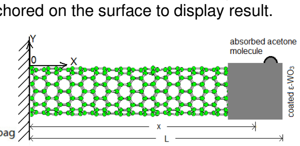


Figure 4. Cantilevered nanotube resonator with an absorbed mass in coated $WO_3$

Piezoelectric activation is used to activate the vibration of carbon nanotube cantilever structure. $W^{6+}$ ions are strong Lewis acid which tends to adsorb acetone molecules: $(CH_3)2C=O+W^{6+}(a)\rightarrow CH_2=C(CH_3)OH+W^{6+}(a)$. When acetone molecules are absorbed by the coated ε-$WO_3$, the resonant frequency of the cantilever will be changed for a certain amount. As shown in Fig. 4, by sensing the resonant frequency change, the existence of a single acetone molecule can be detected by equation of $f=\frac{1}{2\pi}\sqrt{\frac{k}{m_{eq}}}$. By measuring the relative resonant frequency ($f/f_0$), the value of the absorbed acetone can be calculated by equation

$$m_a=[\frac{33}{35(3n^2-n^3)^2}\rho AL+m_{WO3}][\left(\frac{f_{WO3}}{f_a}\right)^2-1]$$, where $m_a$ is the mass of absorbed acetone,

n is defined as n=x/L, ρ, A, L are density cross-sectional area and length of carbon nanotube, $m_{WO3}$ is the mass of coated $WO_3$; $f_a$, $f_{WO3}$ are resonant frequency after acetone absorbed and $WO_3$ coating. The mass of $WO_3$ can be further calculated by

$$m_{WO3}=\frac{33}{35(3n^2-n^3)^2}\rho AL[\left(\frac{f_C}{f_{WO3}}\right)^2-1]$$, where $f_c$ is original resonant frequency of CNT.

The equation can be improved to $m_a=\frac{33}{35(3n^2-n^3)^2}\rho AL\left[\left(\frac{f_C}{f_a}\right)^2-1\right]-m_{WO3}$.

## MATLAB Graphic Analysis

We use Matlab to plot the curves to guide device design. The material properties used are shown in Table 1. Based on above analysis, the relationship between resonant frequency and absorbed acetone mass is shown in Fig 5. As more acetone molecules are absorbed, the resonant frequency of CNT cantilever decreases accordingly.

Table 1. The material parameters used for Matlab plotting

| Parameters | Values |
|---|---|
| Young's modulus $E_{CNT}$ ($ng/nm\cdot s^2$) | $1.0\times10^{15}$ |
| Density $\rho_{CNT}$ ($ng/nm^3$) | $1.4\times10^{-12}$ |
| CNT radius r (nm) | 0.55 |
| CNT length L (nm) | 8 |
| Gravity acceleration g ($nm/s^2$) | $9.8\times10^9$ |
| CNT Poisson's ratio | 0.2 |
| Mass of $WO_3$ $m_{WO3}$ (ng) | $4.95\times10^{-12}$ |
| Width of $WO_3$ (nm) | 1 |
| Thickness of $WO_3$ (nm) | 0.2 |

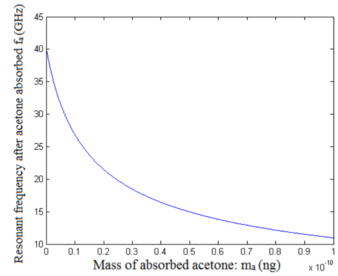


Figure 5. schematic of absorbed acetone and resonant frequency

## ANSYS Simulation Results and Discussion

ANSYS FEM simulation is used to verify the device function. According to the design parameters, the carbon nanotube has the intrinsic frequency of 65.2 GHz without attached mass. The ANSYS simulation gives the same intrinsic resonant frequency (65.2 GHz) as expect by theoretical prediction (Fig 6). 4 cases will be random selected from MATLAB schematic to verify the theoretical model (Fig 7). The ANSYS simulation results are shown in Figure 8-11, the final result comparison is shown in Table 2. As we can see, ANSYS simulation results are in very good agreement with theoretical prediction. This verifies the correctness of our theoretical model.

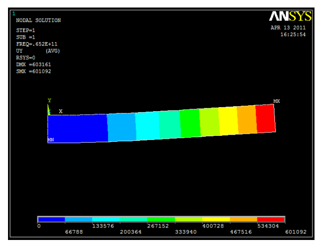


Figure 6. Resonant frequency of CNT when no mass attached (65.2 GHz)

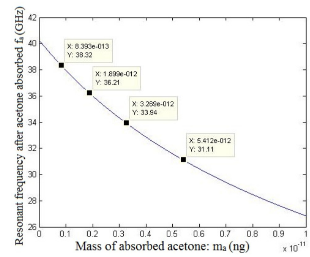


Figure 7. Four points are selected from MATLAB plot for ANSYS verification

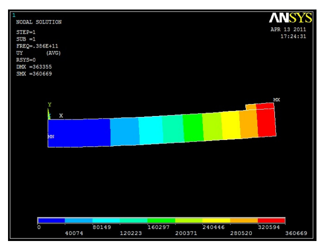


Figure 8. ANSYS frequency simulation for case #1 ($f_1$=38.6 GHz)

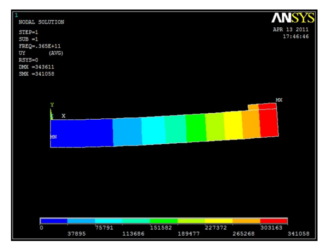


Figure 9. ANSYS frequency simulation for case #2 ($f_2$=36.5 GHz)

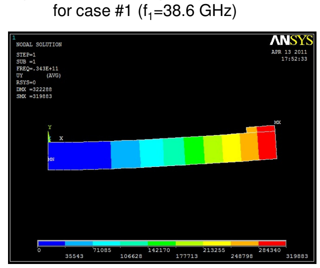


Figure 10. ANSYS frequency simulation for case #3 ($f_3$=34.3 GHz)

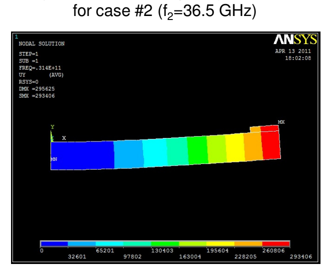


Figure 11. ANSYS frequency simulation for case #4 ($f_4$=31.4 GHz)

Table 2. Comparison between theoretical prediction and ANSYS simulation

| Case # | Absorbed acetone $m_a$ (ng) | Resonant frequency $f_a$ (GHz) (Theoretical) | Resonant frequency $f_a$ (GHz) (ANSYS simulation) | Relative Error |
|---|---|---|---|---|
| 1 | $8.393\times10^{-13}$ | 38.32 | 38.6 | 0.725% |
| 2 | $1.899\times10^{-12}$ | 36.21 | 36.5 | 0.795% |
| 3 | $3.269\times10^{-12}$ | 33.94 | 34.3 | 1.05% |
| 4 | $5.412\times10^{-12}$ | 31.11 | 31.4 | 0.924% |

## Conclusions and Future Work

In this project, the design and theoretical analysis of an ultra-high sensitive breath acetone sensor based on carbon nanotube (CNT) structure is proposed. A theoretical model is developed to describe the vibration of the carbon nanotube cantilever structure. The resonant frequency change of the cantilever due to attached mass is analyzed. The numerical results indicate that the mass sensitivity of carbon nanotube based mass sensor can achieve resolution up to$10^{-26}$ kg. The ANSYS simulation results are in good agreement with theoretical predictions. The proposed acetone sensor can achieve extremely high sensitivity in molecular level. It can be used for non-invasive breath test for diabetes diagnosis. In the future work, we will further focus on the device prototyping and system performance evaluation.