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Performance Enhancement by Implementation of Nanostructure Sensing Element for Bendable SAW Gas Sensor: Simulation

[1]F. Sidek, [1]R. Arsat, [1]Z. Johari, [1]A.A.M Idris and [2]M. Arsat
[1]Faculty of Electrical Engineering,
[2]Department of Technical Education and Engineering, Faculty of Education,
Universiti Teknologi Malaysia (UTM), Johor, Malaysia

Abstract: Flexible technology is current promising area in electronics devices and sensors. There are several advantages such as lightweight, low cost and mechanically flexible which attract the market growth. A rigid Surface Acoustic Wave (SAW) gas sensor that conventionally fabricated on crystals or thin film on substrates is less suitable for uneven surfaces. In addition the interest of applying nanostructure as sensing element has emerged to amplify the performance of the sensors. This study presents comparisons simulation on basic Surface Acoustic Wave (SAW) gas sensor and also the enhanced version by employing nanostructure as a sensitive layer on flexible substrate using COMSOL multiphysics. For the first part, simulation on the sensing element was in thin film form. Next, nanowires were designed and stacked on top of the Inter Digitated Transducer (IDTs), so that it will improve the sensitivity of the gas sensor. In both parts, simulation were done in three different model design condition namely flat, bend in and bend out. The main objective is to investigate the effect of implementing nanostructure as sensing element. The results show increase in sensitivity of the sensor up to 9179.8 kHz/kgm^{-3} and maximum frequency shift of 91.9 Hz after implementing nanostructured.

Key words: Flexible, Surface Acoustic Wave (SAW), gas sensor, simulation, nanostructure, nanowires

INTRODUCTION

Surface Acoustic Wave (SAW) gives excellent performance as a gas sensor for the past 20 years. The surface acoustic wave is exited on a piezoelectric substrate. The nature of acoustic wave generated in the piezoelectric materials is determined by piezoelectric material orientation. The metal electrodes configuration employed purposely to generate the electric field that induces acoustic waves by converse piezoelectric effect. As gas sensors, the SAW devices are coated with layers which selectively absorb analytes of interest and thereby produce a mass change that is then detected through a shift in the resonant frequency of device as shown in Fig. 1 (Kurosawa *et al*., 1990).

In conventional design of SAW gas sensor, the SAW device was fabricated on bulk piezoelectric crystals such as Quartz, LGS, $LiNbO_3$ or $LiTaO_3$, Piezoelectric thin film deposited on rigid substrate (i.e., sapphire or silicon). The advantages provided include technically offer high mechanical and thermal state capability, good frequency response and high electromechanical coupling coefficient (Chen *et al*., 2010; Chiang *et al*., 2012). However, the limitations are complex fabrication and less suitable to be integrated with other devices.

Recently, new interest to develop SAW device with higher performance using flexible substrate. Based on research done by Zhou *et al*. (2012) and Cang-Hai. The result shows the durability of the thin film on flexible polymer produces good electrical stability and resistivity. It changes gradually depends on bending radius. By Jin *et al*. (2013) investigated the performance of flexible SAW device made on nanocrystalline ZnO/polyimide substrate as humidity sensor. In this research, it was found that a high sensitivity of 34.7 kHz/10% Relative Humidity (RH) has been obtained from the flexible device. Their results shows three times igher than those of SAW humidity sensors made on rigid substrates. Bissett *et al*. (2013) investigated and discussed on effect on strain on the chemical functionalization of graphene (used as sensing element). The research demonstrated that graphene can be used to effectively to design and fabricate flexible electronic devices even while being bent and stretch. Understanding the performance of flexible graphene device while undergoing strain contribute of highly sensitive device.

The development to improve the performance had emerged into various phases which include the enhancement of sensing element. It is indeed the most essential process in sensing. The implementation of

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Corresponding Author: F. Sidek, Faculty of Electrical Engineering, Universiti Teknologi Malaysia (UTM), Johor, Malaysia

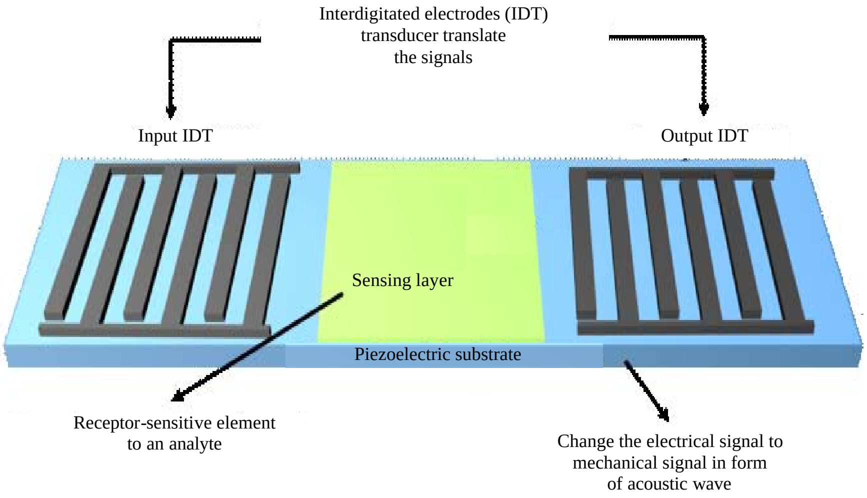


Fig. 1: Surface Acoustic Wave (SAW) gas sensor structure

nanostructures in active area is essential to increase the surface to volume ratio so that, it will enhance the sensitivity of gas sensor.

Nanostructures can be classified into several categories such as dispersed nanoparticles and nanoparticles conjugates, random nanofibers, nanowires, nanotubes, standing nanostructures and porous nanostructures (Tuantranontm, 2012). There are several modelling designs and simulations from the previous works presented by Zhang (2009). These researches were focused on the enhancement of SAW gas sensor sensitivity by implementing nanowires and nanopillars in its active surfaces. Their findings presented that the thickness of nanostructures give a great impact to the sensor sensitivity by reducing the thickness of nanowires into 0.6 μm and by limiting the thickness of nanopillars into 150 nm. Moreover, studies that have been done which involving fabrications produces promising results which employ Zinc Oxide (ZnO) as thin film, carbon nanotubes and Aluminium Nitride (AlN) (Ahmadi *et al*., 2004; Penza *et al*., 2007; Francia *et al*., 2009; Atashbar *et al*., 2009).

The previous researches were focused on flat condition of design. Therefore, this piece of work (presented in this study) focuses on observing the sensor sensitivity towards gas exposure with two configurations. First, adding nanowires as the sensing layer. Second, bending into two different directions to represent flexible state.

This study introduces the modelling techniques which involved including the theory and material used. Next, the details of simulation using COMSOL include the design parameters and details of gas used and the method of sensing. For both part, the results then were discussed in next section and finally conclusion was provided in the end of this study.

MATERIALS AND METHODS

Modelling techniques and simulation: The device was modelled and simulated using finite element simulator COMSOL Multiphysics. This software under the MEMS module has the capabilities to Model Micro Electro Mechanical System (MEMS) by considering the effect of several physical phenomena. This is very important especially when designing sensor where Multiphysics phenomena are utilized for increased function or sensitivity. A typical SAW device consist of delay lines known as Inter Digital Transducer (IDTs) on top of piezoelectric substrate or on thin film which deposited on a substrate as show in Fig. 2.

For both part, three design of SAW sensor investigated are flat, bend in and bend out. Bend in and bend out which represent device bending with degree (h) as in Fig. 3. Zinc Oxide (ZnO) layer was selected as piezoelectric material.

Theory and materials: The propagation of the acoustic waves in a piezoelectric material are based Maxwell's equations (electrical behaviour) and Newton's second law (mechanical behaviour) which provided by Meitzler in Eq. 1 and 2:

$$T_{ij} = C^{E}_{ijkl} S_{Kl} - e_{ijk} E_{k} \tag{1}$$

$$D_{i} = e_{ikl} S_{kl} + \varepsilon^{S}_{ik} E_{k} \tag{2}$$

Where:

T = The stress tensor
c^E = The elasticity matrix
S = The strain tensor
e = The piezoelectric coupling constants
E_k = The electric field intensity
ε^{S}_{ik} = The permeability

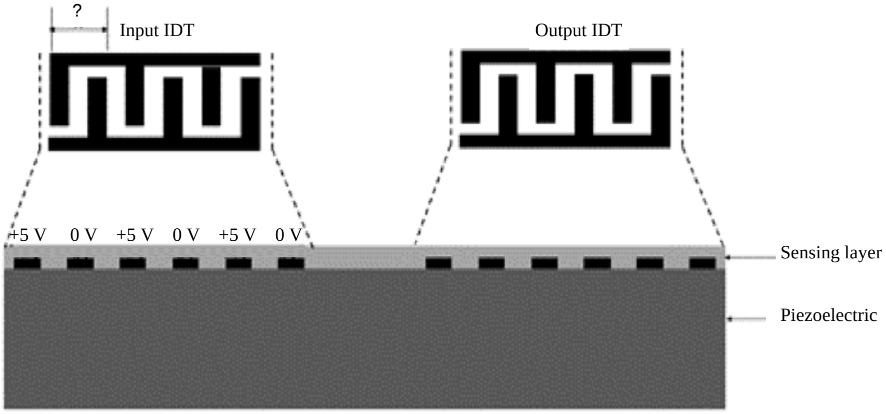
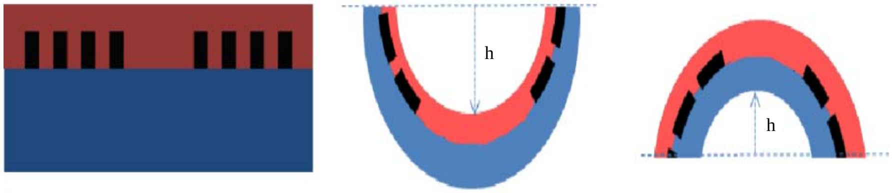


Fig. 2: 2D Geometry setting for SAW gas sensor



Flat

Bend in (concave)

Bend out (convex)

Fig. 3: Three design of SAW gas sensor: flat, bend in and bend out

In order to obtain the optimized SAW device the substrate must have high electromechanical coupling coefficient (k^2) and the acoustic velocity. It determine the amount of electrical wave translated into mechanical in form of acoustic wave. For thin film piezoelectric Zinc Oxide (ZnO) provide high k^2. ZnO is classified as an anisotropic piezoelectric material and the constant of the material are as referred in Eq. 3-5 and summarized in Table 1:

$$c = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & (c_{11}-c_{12})/2 \end{pmatrix} \quad (3)$$

$$e = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & -e_{22} \\ -e_{22} & e_{22} & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix} \quad (4)$$

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix} \quad (5)$$

Table 1: Material constant used for Zinc Oxide (ZnO)

Constants/Symbols	Values
Elastic constant (Pa)	
c_{11}	2.097×10^{11}
c_{12}	1.211×10^{11}
c_{13}	1.055×10^{11}
c_{33}	2.111×10^{11}
c_{44}	4.237×10^{11}
Coupling constant (c/m^2)	
e_{15}	0.480
e_{31}	0.567
e_{33}	2.513
Relative permittivity	
ε_{11}	8.5446
ε_{33}	10.204
Density (kg/m^3)	
ρ	5680

For the Inter Digitated Transducer (IDT) the configuration dimensions has relationship with the wavelength of acoustic wave. Equation 6 define the wave length as:

$$\lambda = 2\left(W_e + W_{sp}\right) \quad (6)$$

Where:

λ = The wavelength
W_e = The width of electrodes
W_{sp} = The space between each electrodes

The operating frequency of SAW device determine by ratio of velocity of wave propagation to the wave length (Bie *et al*., 2007):

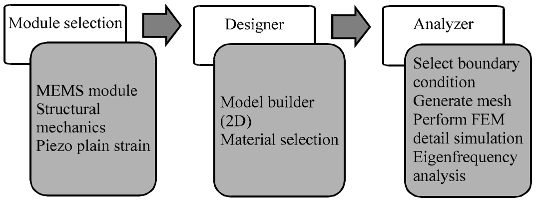


Fig. 4: Simulation step in COMSOL multiphysics

Table 2: SAW gas sensor parameters

Parameters	Dimension (μm)
Periodic distance of IDT fingers (λ)	16.00
IDT finger length (λ/4)	4.00
IDT finger height	0.20
Distance between electrode	1.00
Piezoelectric thickness	22.0
sensing element thickness	0.5
Nanostructured sensing element	0.5×0.1

$$f_0 = \frac{v_0}{\lambda} \tag{7}$$

Simulation using COMSOL multiphysics: In order to analyze the performance of SAW device, simulation finite element Software COMSOL multiphysics was used. The simulation was carried out using 2-Dimensional (2D) piezo Plane Strain Simulation (pzd). The piezo plane strain mode in structural mechanical is used to compute the displacement (Ux, Uy) in the x and y direction and the electrical potential in a plane strain.

For the models simulated, the resonance frequency were investigated. Eigen frequency analysis was performed. The purpose of Eigen frequency analysis is to find the resonant frequency and modes of deformation in the structure. In addition, the wave types can be determined by observing the vibration wave in the structure and comparing it to the wave definition. The highest mechanical displacement was recognized as the mode of interest which has high probability to be the resonant frequency for the SAW. The simulation steps were summarized in Fig. 4.

The design parameters are summarized in Table 2. The sensors employ Aluminum (Al) IDTs etched onto ZnO piezoelectric thin film and covered with Poly Iso Butylene (PIB) thin film and Nanowire Poly Iso Butylene (PIB) as sensing element. The mass of sensing film increases as PIB selectively adsorbs dichloromethane (DCM), CH_2Cl_2 in air. As a result there will be a slight decrease in frequency shift for the sensor. An increase density of PIB sensing film resulting from the adsorption of DCM gas. Air is taken as reference gas and resonance frequency of SAW sensor were exposed to air. When the SAW sensor exposed to 100 ppm of DCM in air at atmospheric pressure and temperature it will results in reduction of resonant frequency. The partial density of DCM in PIB film can be calculated based on Eq. 8 and 9 defined by Ho *et al*. (2003):

$$\rho_{DCM,\ PIB} = K \times M \times c \tag{8}$$

Where:

$K = 10^{1.4821}$ = The air/PIB partition coefficient for DCM
M = The molar mass

$$c = 100 \times 10^{-6} \times p/(RT) \tag{9}$$

Where:

P = The air pressure
R = The gas constant
T = The air temperature

Its rubbery material with Poisson's ratio of 0.48 and Young's modulus of 10 Gpa. For analysis purposes the method to find the frequency shift is as in Eq. 10:

$$\Delta f = f_{(PIB)} \text{-} f_{(PIB+DCM)} \tag{10}$$

An increase density of nanostructured PIB sensing film resulting from the adsorption of DCM gas. When the SAW sensor exposed to 100 ppm of DCM in air at atmospheric pressure and temperature it will results in reduction of resonant frequency.

Sensitivity can be defined as the ratio of the frequency shift in resonance frequency to partial density of the adsorbed in sensing film (Johnson and Shanmuganantham, 2014):

$$\text{Sensitivty} = \frac{\Delta f}{\rho_{PIB+DCM}} = \text{Hz/kgm}^{-3} \tag{11}$$

RESULTS AND DISCUSSION

The sensor performance was analyzed using COMSOL simulation model. Operating frequencies range were between 100-200 MHz. For the first part, thin film sensing element were bend in radius range of 0.2-1.2 μm. Next, resonance frequencies of the enhanced SAW gas sensor were investigated based on the bending radius (h). The bending radius extended of scaled at 1.0, 1.5, 2.0, 2.5 and 3.0 μm. The sensor employed Aluminum (Al) IDTs onto ZnO Piezoelectric thin film and layered with Poly Iso Butylene (PIB) sensing element as illustrated in Fig. 5a-c. Nanowire dimension (width = 0.1 μm and height = 0.5 μm) was defined.

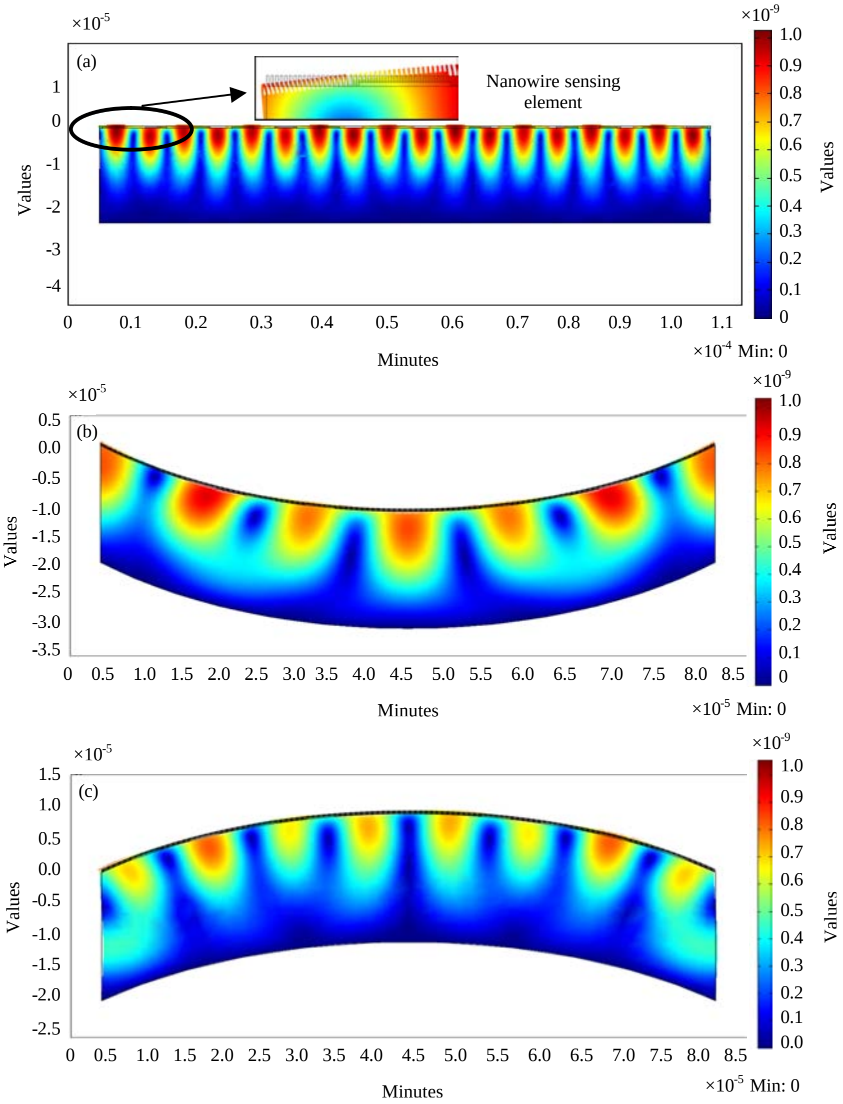


Fig. 5: The deformed shape plot of a free propagating acoustic wave for all three SAW sensor which represent the total displacement of SAW sensor: a) Flat; b) Bend in and c) Bend out

Poly Iso Butylene (PIB) thin film sensing element: Rigid SAW gas sensor produces resonance frequency at 189.5 MHz with maximum total displacement and acoustic velocity of 0.706 nm and 3032.16 m/sec. After DCM gas exposed, frequency shift of 11.1 Hz obtained with sensitivity of 1053.73 Hz/kgm^{-3} determined. The resonance frequency are observed to be decrease with respect to the increasing bending radius. In the range of 189.4 MHz the highest to the lowest value of 82.9 MHz. Improvement have been observed for bend out for radius 0.2 um with frequency shift of 14 Hz and sensitivity of 1324.24 Hz/kgm^{-3} (Fig. 6).

Nanostructured PIB sensing film: The mass of sensing film increases as PIB selectively adsorbs Di Chloro Methane (DCM), CH_2Cl_2 in the air. As a result there will be a slight frequency shift of the sensor. Figure 6 depicts 91.9 Hz of maximum difference in the frequency shifts for bend in and bend out configuration of the sensor. The implementation of nanostructured have affected the sensitivity up to the maximum values of 9179.8 Hz/kgm^{-3} of the sensor due to their increased surface to volume ratio (Fig. 7).

Based on the results obtained there are some comparison can be made based on both design as referred in Table 3. From the resonance frequency it is shown that thin film sensing element was producing greater values compared to nanostructured sensing element. Resonance frequency which produce more stable SAW device if it is near to the theoretical values. Thus, thin film are more

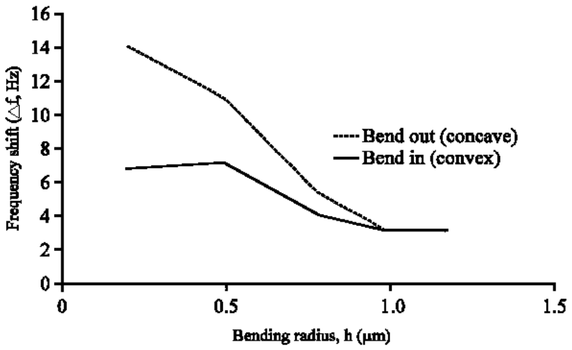


Fig. 6: Bending radius versus frequency shift for PIB thin film as sensing film

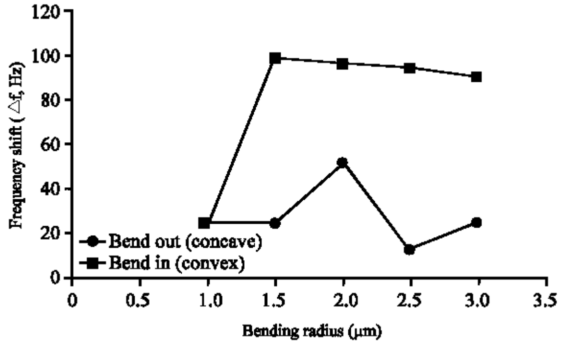


Fig. 7: Bending radius versus frequency shift for nanowired PIB sensing element

Table 3: Comparison for optimum performance for thin film and nanostructured sensing element

Sensing elements structure	Resonance frequency (MHz)	Optimum Δf (Hz)	Optimum sensitivity (Hz/kgm^{-3})
Thin film	189.5	14.0	1324.2
Nanowires	101.5	91.1	9179.8

stable. Next, it was clearly shown that optimum frequency difference (Δf) and sensitivity was higher at nanostructured type of sensing element. These two aspect are essential in providing good performance of a gas sensor.

CONCLUSION

Surface acoustic wave based MEMS gas sensor were simulated in three different design flat, bend in and bend out. For thin film sensing element based on the frequency shift and sensitivity, bend in show the better result which near to flat design with value of 14 Hz and 1324.24 Hz/kgm^{-3}. From the first part of simulation, it shows that the increasing radius h will reduces the operating frequency. Therefore, from this work it is known that certain limit of bending radius h will affect the device performance. In the other hand, the employment of nanostructured have resulted great effect on the frequency shift of 91.9 Hz and sensitivity up to the maximum values of 9179.8 Hz/kgm^{-3} of the sensor due to their increased surface to volume ratio.

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