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Design and simulation of interdigitated electrode for Graphene-SnO$_2$ sensor on acetone gas

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ABSTRACT

This paper presents the design and simulation of interdigitated electrode for graphene-SnO2 sensor on acetone gas. This study focuses on designing and simulating a sensor platform based on IDE with different configuration parameters to obtain the most ideal and efficient layout concerning sensitivity. Eventhough the sensor platform can be easily fabricated by using photolithography, screen-printing and other methods, the simulation is preferable as it provides low cost, secure and quick analysis tools with required sensitivity analysis. The design is important before developing a hybrid gas sensor based on metal oxide and graphene to detect acetone for diabetic mellitus at room temperature. IDE is one of the sensor platforms which provide simplicity, miniaturization and offers an economical mass-fabrication as an alternative to large systems for a sensor. The sensitivity of this IDE can be improved by altering the parameters of the IDE configuration. Herein, COMSOL Multiphysics® 5.4 software is used for simulation where the IDE-based sensor is constructed, and the electrical field is simulated with dependence on several parameters such as width, gap, finger's number and thickness of the electrode. The electrical field that is generated by the simulation results were analyzed and discussed to find the ideal design with the highest sensitivity. From the simulation, it was found that the optimum sensitivity with electrical field of 58808 V/m was the design of IDE configuration with 14 fingers, 0.15 mm spacing size between fingers, 0.15 mm width of the finger and 0.7mm thickness of fingers and electrode.

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1. INTRODUCTION

Volatile organic compound (VOC) is a chemical compound that consists of at least one carbon and one hydrogen atom in its molecular structure that easily evaporate at room temperature [1]. It is classified as one of the most harmful types of pollutants to human health and as according to World Health Organization (WHO), there are two million deaths per year that are caused by poor indoor air quality through the emission of hazardous gases including VOCs [2]. Acetone is one of the common type of VOCs from ketone family [3] and it is present in exhaled breath and used as a biomarker in breath for diabetes mellitus [4]. Diabetes mellitus is a chronic metabolic disorder that arises from insulin deficiency [5-7] that elevates blood glucose levels and is one of the major causes of death. Worldwide, it is estimated that 382 million adults are having diabetes and expected to further increase more than 592millions by 2035 [8].

A healthy person contains less than 0.9 ppm acetone concentration while higher acetone concentration (1.7 ppm–3.7 ppm) is present in the breath of a person with diabetic [9]. As of now, the most generally utilized self-monitoring method to detect diabetes involves the finger-pricking method, an enzymatic-based, and implies the examining of blood sampling from a finger via pricking, to be analyzed by in vitro methods using test strips and a glucometer. Eventhough the test does not give any risk; it is very painful for diabetic patients after doing it several times. The analysis of exhaled air can come up with information on the concentration of acetone and will contribute to an express noninvasive diabetes diagnosis. There are lots of noninvasive method that has been explored to detect and monitor the acetone in exhaled air such as using gas chromatography-mass spectrometry (GC-MS) [10, 11], proton transfer reaction-mass spectrometry (PTR-MS) [9], and Figaro TGS822 [12, 13]. However, they suffer from limitations of cost, portability, and complicated analysis procedure, thus eliminating the possibility of a point of care and real-time diagnosis.

Recently, chemiresistive sensor based on metal oxide semiconductor has been widely used in the gas sensing area because of their ease in fabrication and synthesis, low cost, biocompatibility and high sensitivity [14, 15]. This sensor is used on the detection of various gases such as NO_2 [16], C_2H_2 [17], and VOC [18]. One of the most popular metal oxide materials is SnO_2, which has been extensively used among researchers to detect gases, especially on acetone gas prior to the diabetic mellitus [19] because of its abundant, inexpensive, nontoxicity and high stability [20]. This SnO_2 is hybridized with graphene to increase its sensitivity and improve the response and recovery time [21]. Graphene is a sp^2 hybridization carbon compound with a large surface area of 2630 $m^2\ g^{-1}$, high carrier mobility and thermal conductivity of 250,000 $cm^2 \cdot V^{-1} \cdot s^{-1}$ and 3000 $W \cdot m^{-1} \cdot K^{-1}$ [22, 23]. It also offers a high sensitivity even when operating at room temperature and better long-term stability, although it has a long recovery time. Hybridization of SnO_2 with graphene will help to prevent agglomeration of tin dioxide nanoparticles, which in turn inhibits the restacking of the rGO sheets and enhanced oxygen sorption capabilities [24]. The SnO_2 and rGO n-p heterojunctions also will create an extra depletion region thus improve the sensor response.

Interdigitated electrode (IDE) has been a promising sensor platform as it provides miniaturization of electrodes in a sensor device. This IDE is very convenience as it provides simplicity, cost-effectiveness and the capability of utilizing it on various applications with only minor changes in the sensor configurations usch as the width, length and spacing of the electrode [25]. The structure of the IDE consist of two separate interlocking meshed combs of electrodes, with repetition of configuration. The selection of materials for the electrodes of IDE is also a crucial part as it will affect the sensitivity and reliability of the sensor. The novel metals that are commonly used as an electrode are silver, gold, platinum, and palladium [26, 27]. Among these materials, the most costly material is platinum, yet a very stable electrode material with low degradation and can be used at high temperatures. Even though gold is prominent due to the high reliability and conductivity, however, it is not very suitable for solderation. Silver is the least costly and stable in air. However, under high humidity, it tends to migrate over the surface of resistors. Despite materials selection, the design of the sensor platform itself plays an important role to achieve better and high sensitivity. In real-life, the sensor platform is fabricated by various methods such as photolithography, screen-printing and other methods. The fabrication process needs to go through a few processes like designing, fabricating and validating a prototype, and lastly testing before an ideal design is obtained. This process is time-consuming and not cost-effective as it involved lots of refining and testing work. Hence, this long processes can be avoided by doing simulation before fabricating the sensor platform. Herein, the IDE as a sensor platform is modelled and simulated to optimize the design. The simulation is then interpreted and analyzed to investigate the impacts of the electrode configuration on the overall electrical field.

2. RESEARCH METHOD

This study will focus on the designing of IDE in which the parameters are varied and studied. An IDE layout that consists of two comb electrodes is shown in Figure 1; where L is the length of the finger, G is spacing between fingers, W is the width of the fingers and P is the padding size. Each electrode is connected to +V and −V. The material that has been used for the substrate is alumina while electrode is silver. The properties of these two materials are described in Table 1. A 2D characteristic of the interdigitated electrode sensor is tabulated as in Table 2 for simplicity, and further extend to 3D and the simulation is generated under electrostatics mode of Alternating Current/Direct Current (AC/DC) module in COMSOL Multiphysics® 5.4 software.

The impacts of changing the IDE configuration parameters on the changes in the electrical field were investigated. The electric field is curl free and when the induction is ignored, it is designated by a gradient of voltage (V). The equation for conduction and displacement currents is expressed by [28];

$$-\nabla . [(\sigma + j\omega\varepsilon_r\ \varepsilon_0)\nabla V] = 0 \tag{1}$$

The electrical conductivity is denoted by σ, relative permittivity as ε_r and permittivity of free space as ε_0. (2) and (3) can be obtained from the gradient of voltage (V), electrical field (E) and displacement (D);

$$E=-\nabla V \tag{2}$$

$$D=\varepsilon_r \varepsilon_0 E \tag{3}$$

Four simulations being studied in which the parameters are varied. The design with the highest electrical field on each group of studies will be selected for the simulation on the next parameter. For instance, the first simulation is based on the dependence of the width of fingers which varies from 0.15mm to 0.4mm. After the generation of simulation results, the configuration with the highest electrical field is chosen for the next parameter of simulation. The second simulation is based on the dependence towards gap spacing between fingers which changes from 0.15mm to 0.4mm. The third simulation is based on the dependence on the number of fingers that varies from 8 to 18 fingers while the last simulation is on the dependence of finger thickness which varies from 0.4mm to 0.8mm.

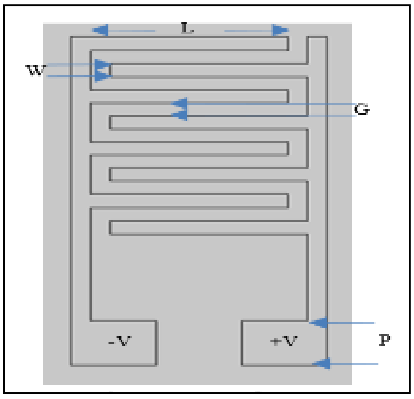

Figure 1. The layout of IDE

Table 1. Properties of alumina substrate and silver as the electrode

	Alumina substrate (Al_2O_3)	Silver (Ag)
Electrical conductivity (S/m)	0	61.6×10^6
Relative permittivity	5.7	-16.5
Coefficient of thermal expansion (1/K)	605×10^{-6}	18.9×10^{-6}
Heat capacity at constant pressure J/(kg. K)	730	235
Density (kg/m^3)	3965	10500
Thermal conductivity w/(m.K)	35	429

Table 2. Parameter of IDE design

Parameter	Values
Electrode and Finger Width, W	Change from 0.15 mm - 0.4 mm Default is 0.3 mm
Electrode Length (L)	8.5 mm
Finger Length	3mm
Spacing between Fingers, G	Change from 0.15 mm - 0.4 mm Default is 0.3 mm
Padding size (P)	1mm x 1mm
Electrode and Fingers thickness	Change from 0.4 mm - 0.8 mm Default is 0.3 mm

3. RESULTS AND ANALYSIS

Figure 2 shows the colormap of the electrical field of the IDE sensor platform that being simulated in COMSOL Multiphysics. The IDE has been simulated based on the dependence of its electrical field in the AC/DC module in COMSOL by varying on the configuration parameters such as IDE width of fingers, the spacing between fingers, number of fingers and finger thickness. It is very important to interpret such parameters for analyzing, and designing IDE in the future.

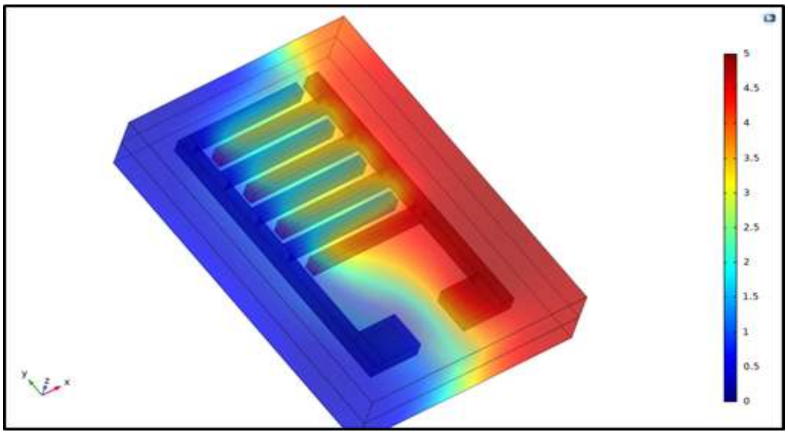

Figure 2. Colormap of the electrical field of interdigitated sensor

3.1. Dependence on the IDE finger width

Different widths of IDE's electrode (0.15mm to 0.4mm) have been computed and simulated. Table 3 and Figure 3 shows the changes in the average electrical field magnitude when the IDE finger widths are changed. It is shown that the IDE finger's width has strongly affected the electrical field of the overall IDE structure. The electrical field decrease with the modification of finger width value from 0.15mm to 0.4mm. The finger with a width of 0.15mm (37865 V/m) is then selected for the next simulation.

Table 3. Average of electrical field magnitude by changing of fingers width

Width of fingers (mm)	Average of electrical field magnitude (V/m)
0.15	37865
0.2	31796
0.25	32267
0.3	30836
0.35	25886
0.4	25162

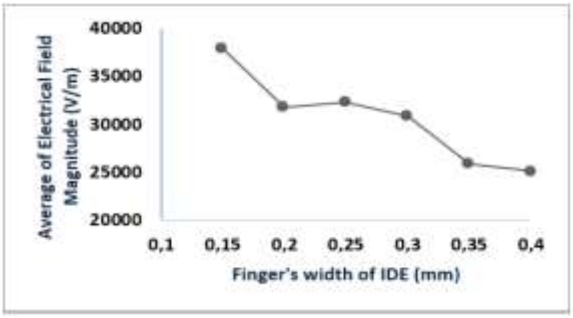

Figure 3. Average of electrical field magnitude by changing of fingers width

3.2. Dependence on the IDE finger spacing

Table 4 and Figure 4 shows the electrical field changes over various IDE finger spacing from 0.15mm to 0.4mm. The experimental results show that the IDE finger spacing gives a strong impact on the overall electrical field as it decreases with the increasing of finger spacing. Next, IDE with the spacing of 0.15mm (33333 V/m) is selected.

Table 4. Average of electrical field magnitude by changing of spacing between fingers

Spacing between fingers (mm)	Average of electrical field magnitude (V/m)
0.15	33333
0.2	25000
0.25	20000
0.3	16666
0.35	14285
0.4	12499

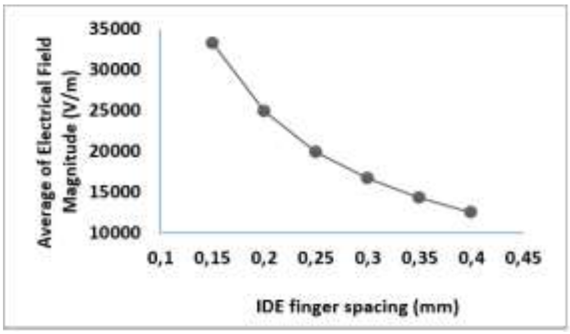

Figure 4. Average of electrical field magnitude by changing of spacing between fingers

3.3. Dependence on the IDE number of fingers

The electric field has been simulated by changing the number of fingers from 8 to 18 on IDE. It is clearly shown in Table 5 and Figure 5 that 14 fingers of IDE reach the highest electrical field (28836 V/m) when the number of fingers is 14.

Table 5. Average of electrical field magnitude by changing of finger's numbers

Number of fingers	Average of electrical field magnitude (V/m)
8	28021
10	28418
12	28438
14	28836
16	28093
18	28225

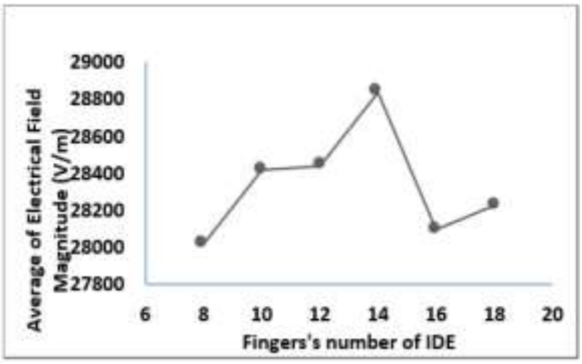

Figure 5. Average of electrical field magnitude by changing of finger's numbers

3.4. Dependence on the IDE finger thickness

It is crucial to evaluate the electrical field of different thicknesses of the IDE finger to investigate the relevance of the finger thickness in designing of IDE. The thickness is varying from 0.4mm to 0.8mm. As shown in Table 6 and Figure 6, the thickness of 0.7mm shows the highest electrical field of 58808 V/m.

Table 6. Average of electrical field magnitude by changing of finger's thickness

Number of fingers	Average of electrical field magnitude (V/m)
0.4	49161
0.5	51233
0.6	48837
0.7	58808
0.8	40666

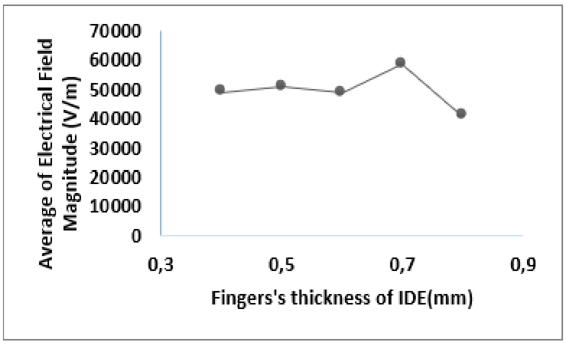

Figure 6. Average of electrical field magnitude by changing of finger's thickness

4. CONCLUSION

A method of simulating the electrical field of IDE was developed using AC/DC module in COMSOL Multiphysics® 5.4 software. In conclusion, these simulations can be used to simulate the effect of the electrical field on the importance of parameters to be considered in the establishment of designing an IDE with higher sensitivity. Under certain conditions, smaller width and interdigit gap/spacing, in general, will lead to higher differences in the electrical field. From the results, the performance of the IDEs can further optimize by selecting the ideal design on the configuration parameters. Significantly, the performance of IDEs is affected by the width of the fingers and spacing between fingers more than finger's numbers. The configuration of IDE with a smaller width of the finger (0.15mm), smaller gap size (0.15mm), 14 number of fingers and thickness of 0.7mm are concluded as the ideal design with the highest electrical field of 58808 V/m. It is also indicating that this design provides a high sensitivity as a sensor platform. These simulations will be further focused on optimizing in maximizing the results in the future with the addition of Graphene-SnO_2 layer on top of the electrodes and to make the IDE design to cope with the devices in the real world and compare the results of simulated design and real devices.

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