Computational Simulation for Interaction between Gold Electrode and Organic Molecule

Tijjani Adam\textsuperscript{1,a}, Mohd Jamilek\textsuperscript{b,2}, and Uda Hashim\textsuperscript{1,c}

\textsuperscript{1}Institute Nano Electronic Engineering, Universiti Malaysia Perlis. (UniMAP),
\textsuperscript{2}School of Microelectronic Engineering, Universiti Malaysia Perlis (UniMAP)
01000 Kangar, Perlis Malaysia
\textsuperscript{a}tijjaniadam@yahoo.com, \textsuperscript{b}mileq_89@yahoo.com, \textsuperscript{c}uda@unimap.edu.com

Abstract—Computational Simulation of Surface Interaction between Organic and Inorganic has been studied by some researchers and much work has been done to elucidate the mechanisms involved in stabilizing the molecule on microstructure and nanostructure but unfortunately, the detailed binding chemistry is still unclear. The study here intended to tackle this problem and the simulation starts by designing the different model with different number of nanowire gold electrode in 3D dimension. Then, design also the model cross section interaction nanowire gold electrode to surface charge as DNA in 2D dimension. After the successful design, the models were simulated using COMSOL software. The electric potential and electric field response for the three models were measured and compared. The electric current will reduce when more number of the nanowire and the electric field will increase when more number of nanowire on gold electrode get in contact.

Keywords— Gold electrode; simulation; organic; DNA molecule; COMSOL Multiphysics 3.5;

I. INTRODUCTION

Gold electrode refers to the electrode nanowire for biosensor application. Gold electrode nanowires are greatly facilities biosensing protocol and the material used is the most favoured because it is reasonably inert. Gold electrodes also obviate the need for a regeneration step so that their future use for decentralised genetic testing can be easily envisioned [1]. In an electrochemical cell, the electrode represents as most important component. It became interface between the electrode and the electron transfers solution of greatest interest occur. To preparing a DNA biosensor is more hard when probe on the surface such as gold electrode for sensing device. The selectivity, sensitivity, accuracy and life of a DNA biosensor directly influence by the amount of immobilized DNA probe. To increase the amount of immobilized DNA greatly, Nano-materials can enlarge the sensing surface area because of excellent biological compatibility and high surface-to-volume ratio.

Before proceed to fabrication process of the device, the simulation model the performance of gold electrode nanowire device is essential. Computer simulation has become an important part of science and engineering. The Digital analytical component, in particular, is important when developing the new products or optimizes the design. Today broad spectrum of available options for simulation; researcher used everything from the basic programming language for advanced packages implement various advanced methods [2]. Simulation is one of the stages that are important before manufacturing device. In simulation, the device can be analysis the optimal functionality and the performance. By using simulation tool, it allows the user produce the prototype even the device become more complex and become more difficult to do experimentally. Simulation program will reduce the time and enable the researcher from the based on the concept of the chip potential and their characteristic performance.

In this paper, the result of gold electrode interaction is observed for the conductance of the device. The simulations of the model design characterized are using COMSOL Multiphysics 3.5.
II. EXPERIMENT PROCEDURE

The geometry model in 3-D made with the different number of nanowire.

![Image](a) (b) (c)

Figure 2. Three different number of nanowire (a) shows the Sub domain Settings and Boundary Settings used to specify each boundary condition of gold electrode nanowire in 3-D; (b) shows the gold electrode nanowire after mesh into small units; (c) shows the figure after Solve the design of gold electrode.

The constant below is for modelling gold electrode interacts with DNA.

<table>
<thead>
<tr>
<th>Name</th>
<th>Expression</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$</td>
<td>300[K]</td>
<td>temperature</td>
</tr>
<tr>
<td>$\epsilon_0$</td>
<td>8.85e-12[F/m]</td>
<td>eps for vacuum</td>
</tr>
<tr>
<td>$\epsilon_{Au}$</td>
<td>10*$\epsilon_0$</td>
<td>Gold</td>
</tr>
<tr>
<td>$\epsilon_{o2}$</td>
<td>4*$\epsilon_0$</td>
<td>oxide</td>
</tr>
<tr>
<td>$\epsilon_{fn}$</td>
<td>25*$\epsilon_0$</td>
<td>Fn</td>
</tr>
<tr>
<td>$\epsilon_{el}$</td>
<td>80*$\epsilon_0$</td>
<td>$\epsilon_{el}$</td>
</tr>
<tr>
<td>$e$</td>
<td>-1.602e-19[C]</td>
<td>Electronic charge</td>
</tr>
<tr>
<td>$\sigma_{34}$</td>
<td>-40.0E11<em>e</em>100*100</td>
<td>surface charge at bnd34</td>
</tr>
<tr>
<td>$k_B$</td>
<td>1.23e-23[J/K]</td>
<td>Boltzmann constant</td>
</tr>
</tbody>
</table>

The geometry modelling in 2-D cross section of gold electrode interact with DNA is made as Fig.3 below.

![Image](a) (b) (c)

Figure 3. Show the model in 2-D of interaction gold electrode to DNA

The models of the interaction nanowire boundary are including the electrode nanowire, a thin layer of amino, functional layer and surrounded by an electrolyte [4]. The biosensor under consideration consisted of nanowire gold electrode with radius 40nm surrounded by 2nm amino layer and 5nm thick of functional bio-interface layer surrounded of the amino layer and thickness of the electrolyte was set to 200 nm and thus distance of Dirichlet boundary $|\Omega| = 222$ nm. Surface charge densities for Neumann boundary conditions were set as follows.

$\sigma_{12} = 0, \sigma_{23} = 0$ and $\sigma_{34} = -3.3642e-4$ C/m.

The model geometry 2D will design to reduce computation and memory requirements by using COMSOL software. Using COMSOL software, the mode application used to interact between them is Partial Differential Equation (PDE), general form (g).

![Image](a) (b) (c)

Figure 5. Resistance v/s Permittivity increases as the wire reduced in sizes

Figure 6. Show the model interaction gold electrode with DNA

Figure 7. Resultant response of the device with respect to the number of wire number.

From the Fig.5 above, show the design interaction gold electrode to surface charge as the DNA. In Fig.4 also shows potential distribution on a cross-section perpendicular to the nanowire gold electrode axis, from the picture there is non-negligible potential inside gold nanowire due to surface charge at the interface $\Omega_{34}$ between functional bio-interface and the electrolyte.
III. RESULT AND DISCUSSION

The capillary flow experiment in different number of gold electrode nanowire and it interaction to surface charge as DNA was used COMSOL Multiphysics software. The experiment have been conducted using Electrostatic (emes) and Conductive media DC (emdc) for simulating the different number of nanowire design model. Then, experimental of gold electrode nanowire interaction to DNA using Partial Differential Equation (PDE-general form,g) for the model design simulated. From experiment simulation of the three geometry model, each model contributes the different electric potential. Then, the result was compared.

![Figure 8. Comparing Graph characterize of electric potential.](image)

The result of the electric potential for single, double and triple design model is compare as shown in fig. 6. From the graph chart, the result of electrical potential will reduce when the number of wire for the model design is increased. The potential of current reduce by increasing number of wire because the resistance on the nanowire become parallel when the number of nanowire increasing. In theoretical, the resistor of the parallel circuit has a low resistance compare to single resistor. When the resistance is low, so that the voltage supplies will be low to conducting the current flow on the nanowire.

The theory of Ohm’s Law stated that the voltage is proportional to current when the resistance is constant. The Ohm’s Law state as formula below.

\[ V = IR \]

From the Ohm’s Law, when the resistance is reduce the voltage apply also reduce for conducting the current to flow on the nanowire.

![Figure 9. Graph characterize of electric field norm vs. arc-length](image)

(a) One electrode nanowire (b) two electrode nanowire (c) three electrode nanowire

All the Three designs were tested using electric field norm and it has been found out that the designed the graph in fig.7(c) with three wires is more suitable because the electric field is higher. Here there is not all that obvious however, the result enlarged the scale in order to show more detail. The absolute of electric field norm maximum were in 1.5e5 V/m. The methodology for finding the optimal configuration is easily summarized. For given boundary data in fig.7(c) compute the electric field response solution for which the device produced the highest. Then place each wire in parallel inside subdomains with boundaries given by the equipotential of V and here is well known fact that when two resistance are brought together the individual resistance reduce. This might the cause of getting response in model in fig. 8 and 9. From the fig.4, the different potential distributed on the gold electrode nanowire produce by seeing the colour of range potential. That mean has a some different potential on the nanowire to surface by links to other layer. The results can be obtained in the form of graph from cross-section plot parameters after post processing and visualization steps. After post-processing the design model, ultimately result change in conductance of the nanowire due to change in surface charge at the surface is shown in fig.4. From that result, can notice that the curve is nearly linear around \( \sigma_{34} \to 0 \) and the curve starts to deviate from linearity when \( \sigma_{34} \) gets larger.

![Figure 10. Simulation software using COMSOL Multiphysics 3.5. The potential nonlinear dependence of gold electrode nanowire conductance on the surface charge \( \sigma_{34} \).](image)

From the fig.5,6,7 show that the graph conductance increasing when the more interaction on the surface charge to nanowire gold electrode. More charge of DNA that interacts to gold electrode nanowire will increase the current flow by applying the same voltage to the gold electrode nanowire. The DNA molecule have some charge, when it bind to the linker, it will produce the current fig.10. When the current flow combines to the current charge from DNA, it produces more current flow.

IV. CONCLUSION

The presented a design, simulation and characterization the interaction gold electrode nanowire in two-dimensional is achieved. COMSOL Multiphysics 3.5 used to get a better understanding of the characteristic of gold electrode nanowire with different number and it interaction to the surface charge like DNA. The three-dimensional of gold...
electrode nanowire are simulating to determine the different potential and the electric field from the three geometry model that solving using electrostatic (emes) and conductive media DC (emdc). Then, the design in two-dimensional of interaction gold electrode nanowire with surface charge as DNA are simulate to determine the conductance when both of them are interact. The design model simulation was done in COMSOL Multiphysics 3.5 by first solving the partial differential equation (PDE), general form (g). Increasing the number of nanowire for biosensor will increase the capability of the current flow and increasing the surface charge to gold electrode nanowire was increase the conducting current flow by supply the same voltage.

ACKNOWLEDGMENT

Here, the authors like to thank Universiti Malaysia Perlis (UniMAP) and Ministry of Higher Education Malaysia for giving FRGS grant to conduct this research in the Micro & Nano Fabrication Lab. Do not forgetting to all members of the group in the Institute of Nano electronic Engineering especially the Nano structure Research Group.

REFERENCES

[27] Tijjani Adam, U. Hashim, Ultra thin polysilicon layer formation: Statistical process optimization by Taguchi's technique


