JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 11 No 1, 01005(5pp) (2019)
ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 11 № 1, 01005(5cc) (2019)

Simulation Study of Field-effect Transistor Based Cylindrical Silicon Nanowire Biosensor: Effect of Length and Radius of the Nanowire

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(Received 12 October 2018; revised manuscript received 04 February 2019; published online 25 February 2019)

In the present report, we have simulated the FET based silicon nanowire biosensor and studied the effect of nanowire length and radius on the different functional characteristics of the silicon nanowire biosensor. We have used *BioSensorLab* open source simulation tool for the present investigation. Particularly, we have studied the effect of nanowire length and radius on conductance modulation with respect to target molecule density, conductance modulation with respect to buffer ion concentration, nanowire surface potential with respect to *pH*, signal to noise ratio (SNR) with respect to receptor density, settling time with respect to analyte concentration and density of captured molecule with respect to detection time. We have taken into account the electrostatic interaction between receptor molecules and target biomolecules, which is based on the Diffusion-Capture model. The results suggested that the higher conductance modulation can be achieved at the higher target molecule density with a larger radius of the silicon nanowire. On the other hand, maximum conductance modulation is observed at the lower radius of the silicon nanowire with lower buffer ion concentration. The simulation results suggested that the surface potential of the nanowire tends to decrease as the *pH* increases for both cases (nanowire length and radius). No significant effect on the signal to noise ratio due to the change in the nanowire length and radius was observed. It is observed that the nanowire length does not affect the settling time; however, change in the nanowire radius shows the significant effect on the settling time. In the nutshell, the nanowire length and radius significantly affect the performance parameters of the FET based silicon nanowire biosensor.

Keywords: Nanowire, Biosensor, FET, Simulation.

DOI: 10.21272/jnep.11(1).01005 PACS numbers: 62.23.Hj, 87.85.fk, 31.15.xv

1. INTRODUCTION

In recent years, numerous types of biosensors have attracted a lot of attention for the point-of-care diagnostic application [1]. The biosensor is a sensing device or a measurement system specifically designed for the estimation of unknown materials. The estimation can be achieved with the help of biological interactions. In addition to this, these interactions can be converted into the electrical signal representation for the immediate reading, storing, and further processing purpose. In general, signal transduction and biorecognition elements (bioreceptors) are the basic building block by which we can differentiate the different types of biosensors. The nucleic acids, antibodies, cells, enzymes, etc. can work as biorecognition elements or bioreceptors. In the nutshell, the biorecognition element identifies/reacts to the target system and finally electronic circuitry converts the biological signal into its electrical equivalent. Moreover, the biological signal representation can be also possible with the help of optically, acoustically, mechanically, and calorimetrically [2].

In recent years, field-effect transistor (FET) based silicon nanowire biosensors have attracted a lot of attention due to its superior sensitivity. Silicon nanowire FET based biosensors having functional biointerface which consists of receptor molecules and plays a key role in the detection of target biomolecules [3]. Recently, Adam and Hashim [3] have reported the silicon nanowire liquid gate control based sensor device. The developed sensor can work as ultra-sensitive pH sensor and detect specific DNA or protein molecules [3]. Nuzaihan et al. have developed a novel molecular gate control based silicon nanowire biosensor. The developed biosensor can detect the DNA of the dengue virus. The reported biosensor can be useful for the point-of-care diagnostic applications [4]. Azmi et al. have reported the functional device based on silicon nanowire biosensor for detection of cancer risk biomarker. The developed biosensor detects the biomarker 8-OHdG [5]. A good review article based on the silicon nanowire biosensor can be found in the ref. [6].

In the present report, we have simulated the FET based silicon nanowire biosensor and studied the effect of nanowire length and radius on the different functional characteristics of the silicon nanowire biosensor. Particularly, we have studied the effect of nanowire length and radius on (i) Conductance modulation and target molecule density of silicon nanowire biosensor; (ii) Conductance modulation and buffer ion concentration of silicon nanowire biosensor; (iii) Nanowire surface potential and pH of silicon nanowire biosensor; (iv) Signal to noise ratio (SNR) and receptor density of silicon nanowire biosensor; (v) Settling time and analyte

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concentration of silicon nanowire biosensor; (vi) Density of captured molecule and detection time of silicon nanowire biosensor.

2. COMPUTATIONAL DETAILS

In the present investigation, we have used *BioSensorLab* which is available at the Nanohub website for the simulation of FET based silicon nanowire biosensor [7]. It is a numerical simulator developed for the prediction of performance parameters of different kinds of electronic biosensors. It is based on the principle of electrostatic interaction between receptor molecules and target biomolecules and modeled around the Diffusion-Capture model [8]. The FET based silicon nanowire biosensor consists of source and drain terminals and silicon nanowire is attached to source and drain terminals. The surface of the silicon nanowire is functionalized with the receptor molecules in order to detect the target biomolecules. Most of the biomolecules have intrinsic electrostatic charge capability, hence electrostatic interaction between receptor molecules and target biomolecules occurs. This can affect the distribution of the electrostatic potential throughout the nanowire and conductance (current) of the nanowire is varied in accordance with the electrostatic interaction between receptor molecules and target biomolecules [7-8]. In the end, the variation in the resultant current can be measured by applying a voltage across the source and drain terminals [9]. The simulation parameters of the FET based silicon nanowire biosensor are as follows, oxide thickness: 1 nm, doping density: $1e^{19}$/cc, lower value of analyte concentration: $1e^{-15}$ M, upper value of analyte concentration: $1e^{-6}$ M, No. of intermediate concentration steps: 30, minimum no. of molecules: 10, surface density: $5e^{14}\ cm^{-2}$, protonation constant: -2, de-protonation constant: 6, lower value of electrolyte concentration: 1e-5 M, upper value of electrolyte concentration: 2 M, size of the receptor molecule 2 nm; size of the parasitic molecule: 1 nm, concentration of target molecule: $1e^{-12}$ M, concentration of parasitic molecule: $1e^{-6}$ M, maximum surface coverage: 0.54, lower value of receptor density: $1e^{11}\ cm^{-2}$, and lower value of receptor density: $5e^{12}\ cm^{-2}$.

3. RESULTS AND DISCUSSION

In this investigation, we have varied the nanowire length as 100 nm, 1 μm, 10 μm, and 100 μm. Furthermore, we have also varied the nanowire radius as 10 nm, 20 nm, 30 nm, and 50 nm. Particularly, we have studied the effect of nanowire length and radius on (i) Conductance modulation and target molecule density of silicon nanowire biosensor; (ii) Conductance modulation and buffer ion concentration of silicon nanowire biosensor; (iii) Nanowire surface potential and *pH* of silicon nanowire biosensor; (iv) Signal to noise ratio (SNR) and receptor density of silicon nanowire biosensor; (v) Settling time and analyte concentration of silicon nanowire biosensor; (vi) Density of captured molecule and time of silicon nanowire biosensor. The effect of nanowire length and radius on conductance modulation and target molecule density of FET based silicon nanowire biosensor is shown in Fig. 1. The results suggested that the conductance modulation increases as the target molecule density increases. It is observed that the conduction modulation rapidly increases after 10^{-8} molar density for both cases (nanowire length and radius). It is observed that the nanowire having length 1 μm shows higher conduction modulation than other counterparts. In addition to this, other nanowires (100 nm, 10 μm, and 100 μm) do not show any significant change in the case of the conductance modulation. On the other hand, conductance modulation tends to increases as the radius of the silicon nanowire increases from 10 nm to 50 nm. The conductance modulation is not always proportional to the target molecule density. This is due to fact that the nonlinearity in the electrostatic screening which is a presence in the counter ions in the electrolyte solution [10]. In view of this, higher conductance modulation can be achieved at the higher target molecule density with a larger radius of the silicon nanowire. This is due to fact that a larger nanowire radius provides a higher surface to detect the target biomolecules.

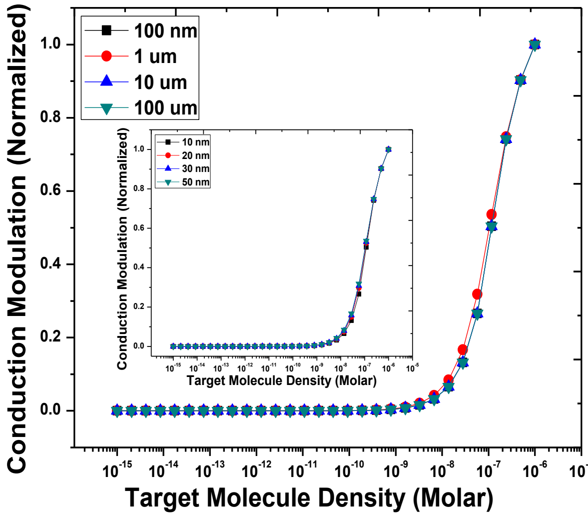

Fig. 1 – Effect of nanowire length and radius (inset) on conductance modulation with respect to target molecule density of silicon nanowire biosensor

The effect of nanowire length and radius on conductance modulation and buffer ion concentration of FET based silicon nanowire biosensor is shown in Fig. 2. The results suggested that the conduction modulation exponentially decreases with increasing buffer ion concentration for both cases (nanowire length and radius). It is observed that the nanowire having length 1 μm shows lower conduction modulation than other counterparts with respect to buffer ion concentration. In addition to this, other nanowires (100 nm, 10 μm, and 100 μm) do not show any significant change in the case of the conductance modulation. In the case of nanowire radius, conductance modulation tends to decreases as the radius of the silicon nanowire increases. In the nutshell, the maximum conductance modulation is observed at the lower radius of the silicon nanowire with lower buffer ion concentration. This may be due to the higher surface to volume ratio observed at the lower radius of the silicon nanowire. The effect of nanowire length and radius on surface potential with respect to

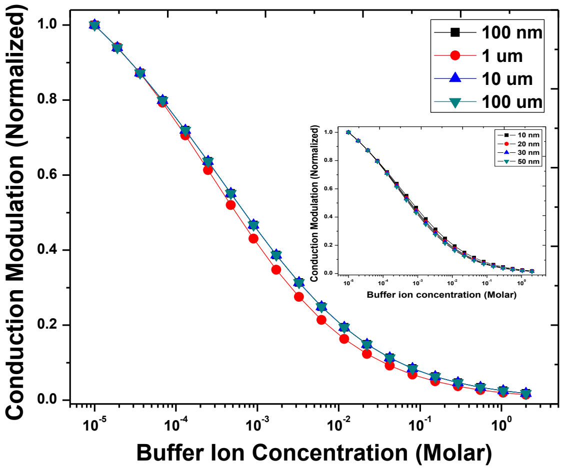

Fig. 2 – Effect of nanowire length and radius (inset) on conductance modulation with respect to buffer ion concentration of silicon nanowire biosensor

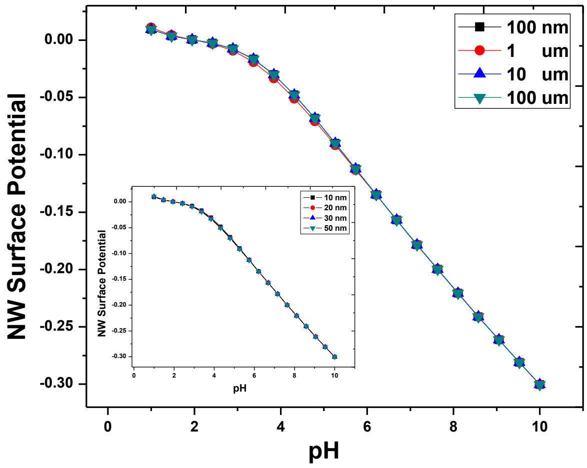

Fig. 3 – Effect of nanowire length and radius (inset) on nanowire surface potential with respect to *pH* of silicon nanowire biosensor

different *pH* is shown in Fig. 3. It is observed that the surface potential of the nanowire tends to decrease as the *pH* increases for both cases (nanowire length and radius). It is interesting to note that the surface potential of the nanowire steadily increases (lower slope) at lower *pH* value and abruptly increases at higher *pH* value (higher slope). It is observed that the nanowire having length 1 μm shows lower surface potential than other counterparts with respect to *pH*. In addition to this, other nanowires (100 nm, 10 μm, and 100 μm) do not show any significant change in the surface potential with respect to change in *pH*. In the case of nanowire radius, the surface potential tends to decrease as the radius of the silicon nanowire increases. The simulation results are in good agreement with the experimental results reported in the Ref. [11].

The signal-to-noise ratio is one of the performance parameters of the FET based silicon nanowire biosensor and it should be as high as possible. The higher signal to noise ratio suggested the FET based silicon nanowire biosensor detects the desired target molecule and rejects the parasitic molecules. The effect of the nanowire length and radius on signal to noise ratio with respect to different receptor density is shown in Fig. 4. The nanowire length and radius do not show any significant effect on the signal to noise ratio. In the other words, change in the length and radius of the silicon nanowire does not show any significant effect on the signal to noise ratio. However, results clearly suggested that the signal to noise ratio of the FET based silicon nanowire biosensor tends to increase as the receptor density increases. It is interesting to note that the signal to noise ratio shows the exponential increasing behavior for both cases (nanowire length and radius). This is due to fact that the diffusion limited transport mechanism is generally observed at the lower receptor density, and strength of the signal becomes strong at the higher receptor density [12]. The increase in the signal to noise ratio at the higher receptor density is due to the decrease in the surface voids. The decrease in the surface voids reduces the adsorption of the parasitic molecule on the surface of the sensor. This results in the increase in the density of conjugated target-receptor, which increases the wanted signal and reduces the noise in the detected signal [12].

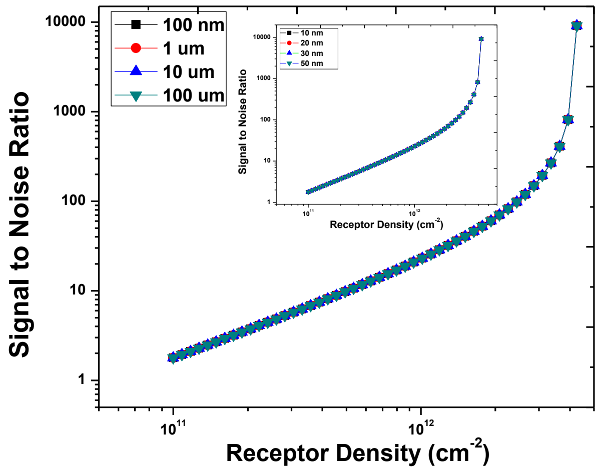

Fig. 4 – Effect of nanowire length and radius (inset) on signal to noise ratio (SNR) with respect to receptor density of silicon nanowire biosensor

The settling time represents the time taken by a target biomolecule to reach the sensor surface. The effect of nanowire length and radius with respect to an analyte concentration of silicon nanowire biosensor is shown in Fig. 5. The results suggested that the settling time decreases as the analyte concentration increases. It is observed that the nanowire length does not affect the settling time, however, change in the nanowire radius shows the significant effect on the settling time of the silicon nanowire biosensor. It is observed that the settling time tends to increase as the radius of the nanowire increases from 10 nm to 50 nm. The decrease in the settling time at the higher analyte concentration is due to the weakening of diffusion-limited transport. Considering the above trend, we have simulated the silicon nanowire biosensor and studied the time domain performance with respect to change in the nanowire length and radius, as shown in Fig. 6. It is observed that the density of captured molecule increases as a function of detection time. The linear change in some duration of time and becomes saturated after some time.

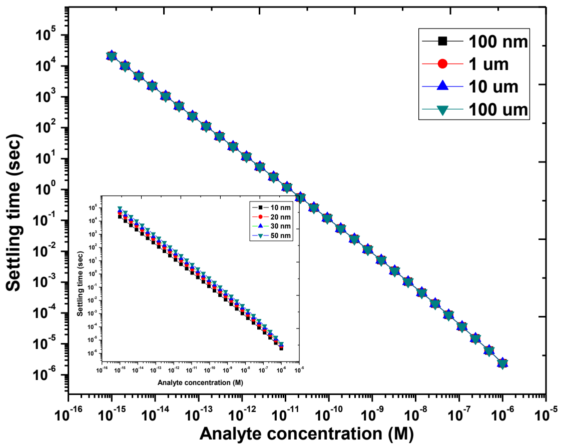

Fig. 5 – Effect of nanowire length and radius (inset) on settling time with respect to an analyte concentration of silicon nanowire biosensor

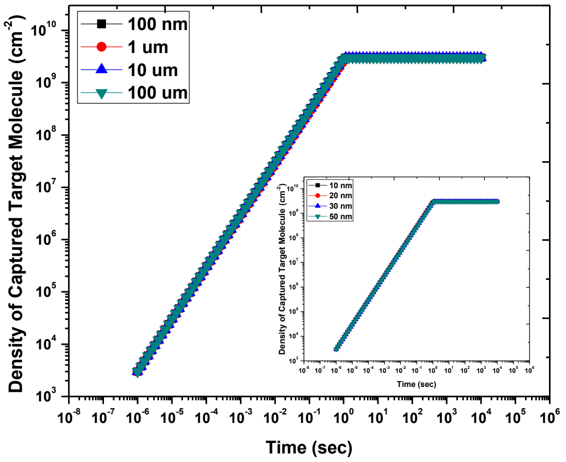

Fig. 6 – Effect of nanowire length and radius (inset) on the density of the captured molecule with respect to the time of silicon nanowire biosensor

This phenomenon arises due to fact that the target molecules are very close to sensor surface at the beginning, hence target molecules can be captured at the very short time. As time progresses, the density of the captured molecule increases which increases the detection time of the sensor. The saturation observed in the density of the captured target molecule at a longer time is due to the balance of forward and backward reactions [13].

4. CONCLUSIONS

The present report deals with the simulation study of FET based silicon nanowire biosensor and investigated the effect of nanowire length and radius on the different functional characteristics of the silicon nanowire biosensor. The results suggested that the conductance modulation increases as the target molecule density increases. On the other hand, conductance modulation also increases as the radius of the silicon nanowire increases from 10 nm to 50 nm. In view of this, higher conductance modulation can be achieved at the higher target molecule density with a larger radius of the silicon nanowire. Furthermore, conduction modulation exponentially decreases with increasing buffer ion concentration for both cases. It is observed that the surface potential tends to decrease with increase in the *pH*. It is interesting to note that the surface potential of the nanowire steadily increases (lower slope) at lower *pH* value and abruptly increases at higher *pH* value (higher slope). The nanowire length and radius do not show any significant effect on the signal to noise ratio. However, results clearly suggested that the signal to noise ratio of the FET based silicon nanowire biosensor tends to increase as the receptor density increases. Furthermore, the signal to noise ratio shows the exponential increasing behavior for both cases. In addition to this, the settling time decreases as the analyte concentration increases. It is observed that the nanowire length does not affect the settling time; however, change in the nanowire radius shows the significant effect on the settling time of the silicon nanowire biosensor. It is observed that the settling time tends to increase as the nanowire radius increases from 10 nm to 50 nm. The decrease in the settling time at the higher analyte concentration is due to the weakening of diffusion-limited transport. Furthermore, the density of captured molecule increases as a function of detection time. The linear change in the density of the captured molecule is observed for some duration of time and becomes saturated after some time. The saturation observed in the density of the captured target molecule at a longer time is due to the balance of forward and backward reactions.

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Моделювання біосенсора у вигляді циліндричного кремнієвого нанодроту на основі польового транзистора: вплив довжини і радіусу нанодроту

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У даній статті ми моделювали біосенсор у вигляді кремнієвого нанодроту на основі польового транзистора і вивчали вплив довжини та радіусу нанодроту на різні функціональні характеристики біосенсора. Для цього дослідження ми використали інструмент моделювання BioSensorLab з відкритим вихідним кодом. Зокрема, ми вивчали вплив довжини і радіусу нанодоту на модуляцію провідності по відношенню до щільності молекул-мішеней, модуляцію провідності щодо концентрації буферних іонів, варіацію потенціалу поверхні нанодроту щодо *pH*, зміну відношення сигнал/шум щодо щільності рецептора, варіацію часу осадження щодо концентрації і зміну щільності захопленої молекули щодо часу виявлення. Ми взяли до уваги електростатичну взаємодію між молекулами рецептора і біомолекулами-мішенями, що базується на моделі дифузійного захоплення. Результати показали, що більш високу модуляцію провідності можна досягти при більш високій щільності молекул-мішеней з більшим радіусом кремнієвого нанодроту. З іншого боку, максимальна модуляція провідності спостерігається при меншому радіусі кремнієвого нанодроту з меншою концентрацією буферних іонів. Результати моделювання показали, що поверхневий потенціал нанодроту має тенденцію до зменшення, оскільки величина *pH* зростає в обох випадках (довжина і радіус нано-дроту). У свою чергу, істотного впливу на відношення сигнал/шум через зміну довжини і радіусу нанодроту не спостерігалося. Було також виявлено, що довжина нанодроту не впливає на час осадження, проте на нього значним чином впливає зміна радіуса нанодроту. Таким чином, довжина і радіус нанодроту суттєво впливають на робочі параметри біосенсора на базі польового транзистора.

Ключові слова: Нанодріт, Біосенсор, Польовий транзистор, Моделювання.