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Design and Analysis of Silicon Nanowire FET for the Detection of Cardiac Troponin I Biomarker

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Abstract

Cardiac arrests are one of the major health problems in present days. Cardiac Troponin-I (cTnI) is one of the important enzymes that causes cardiac arrest. Early diagnosis and proper medication of this saves human life. One of the prominent devices to diagnose troponin I is FET based bio-sensor. Normally, for these sensors' higher sensitivities will be obtained as these biosensors structure consists of nanowire FETs. Proper selection of materials, dimensions, and doping concentrations of nanowire FET imply the perfection of a nanowire FET-based biosensor. In this work, Silicon Nanowire (SiNW) FET sensor is designed and simulated using COMSOL Multiphysics. Through this design, Identified the presence of different concentrations of cTnI present in human blood. The presence of different enzymes like cTnT, cTnI etc., bring changes in characteristics of SiNW FET sensor. With these changes in characteristics, we can identify the presence of these enzymes of a lower concentration also. The lower concentrations of these biomarkers will bring notable changes in the drain current. The characteristics were analysed with the SiNW FET which is equipped with immobilized antibodies on it. The considerable changes observed in these characteristics of FET sensor identifies the presence of cTnI biomarker and are attached to the monoclonal Antibodies (mAb). Our observations shown that the properties of designed SiNW FET changes with presence of these bio marker materials and a limit of detection is obtained the order of 2pg/mL. with further the design bio sensor with SiNW FET can be used for microfluidic and Lab-on-Chip applications also.

Keywords: SiNW FET, bio-sensor, monoclonal Antibody, cTnI, bio-marker materials.

1: Introduction

Nanotechnology turns out to be one of the vital things in our day-to-day life which includes bio-medical applications too. Major bio medical applications comprise bio-sensors. These bio-sensors are greatly desirable for the early detection of the lethal diseases. These sensors are the analytical devices integrated with molecular recognition and sensing materials. The detection principle in sensors is subjected to the interaction between its target and the recognition molecule. Sensitivity of the sensors is the foremost criterion for sensor designing. SiNWs can be used as one of the prominent devices for the implementation of bio-sensors due to their high surface to volume ratio and high chemical reactivity [1,2]. SiNW provides higher sensitivity than bulk FETs. Because SiNWs acts as gate in a nanowire FET. SiNW FETs are also used for the detection of ultra-low concentrations of biomolecules [3,4].

Nanowires are similar in size when compared to cells, proteins which allow them to associate with them that further brings some characteristic change in the Nanowire devices. Sensing devices comprised of nanowires with reduced lengths exhibited higher sensitivity than nanowires with greater lengths so the device sensitivity depends on the channel dimensions and doping concentration [5]. The brilliant feature of nanowire FETs is the binding of a charged element on their surface brings computable variations in their conductivity. This variation in the

conductivity over the nanowires carries further a change in the current through them as these nanowires offer a high surface to volume ratio (S/V). The sensitivity of these biosensors is certainly high while they function at room temperature. The sensitivity of nanowire-based sensors can spot the level to micromoles and show quicker response time [3,6]. The raise in drain current enhances the sensitivity value. The resistance of nanowires has a key influence on the sensitivity of the nanowire. Nanowires with more lengths and narrower widths provide higher sensitivity towards immunodetection. The sensitivity of these sensors also affected by the variation of the surface potential voltage between the electrolyte edge and the sensing layer [7,8]. The highest current and conductance values are attained for intrinsic SiNW-based sensors in contrary to impure SiNW-based FET sensors. Another great advantage of pure silicon-based FET sensor is the noise generated by impurities is condensed compared to doped nanowire-based sensor. Which is suitable for the production of reliable SiNW FET based biosensors [9,10].

There achieved an abundant progress in the production of ultrasensitive nano-sensors for biochemical analysis, high sensitivity, detection of biological molecules and several other unique properties [11,12]. It has been proven for the extremely sensitive detection; SiNWs can be used as Bio-FET. To detect biological entity, we should make the surface prone. It is shown that the nicotine-streptavidin is used as prototype. With the help of micro fluid approach, we can have environmental control. Along with automated custom-built micro fluid platform SiNW can be represented controlling the chemical handing and data analysis. The main disadvantage is the cost per chip required for the fabrication process. For the detection of antibodies, micro fluid set-up can be built. Depending upon the design of nanowire, the sensitivity is measured. The main objective is to measure nanowire resistance over time in various ranges of voltage [13].

In this paper we designed a SiNW FET sensor which has the capability to identify the presence of cTnI biomarker with lower concentrations when compared to a normal range of cTnI.

2: Design and analysis of Silicon nanowire FET sensor

In COMSOL Multiphysics the semiconductor, chemical reaction and transport of diluted species modules were used to design and simulate a SiNW FET biosensor. The structure of proposed design was shown in the Figure1(a). The device structure consists of a SiNW surrounded by an oxide layer. The oxide layer acting as a dielectric layer with a dielectric constant of 3.9. Drain and transfer characteristics were calculated for the analysis of the response. These characteristics were obtained by varying channel dimensions, doping concentrations and parameters of the device. With the proposed designed structure, we allowed the drain current to conduct only through nanowire no other conducting channel exist between source and drain with which can easily understand the behavioural characteristics of the SiNW.

SiNW present in the proposed structure behaves as channel for the conduction between drain and source. As it is semiconductor in nature it won't allow current at room temperature. To improve the conducting current value, we dope it with impurities. The doping concentration will play significant role in the current conduction. Normally, doping of silicon can be done with two different types of dopants i.e., acceptors and donors. By way

of the mobility of electrons is more, we prefer doping of nanowire with V group elements.

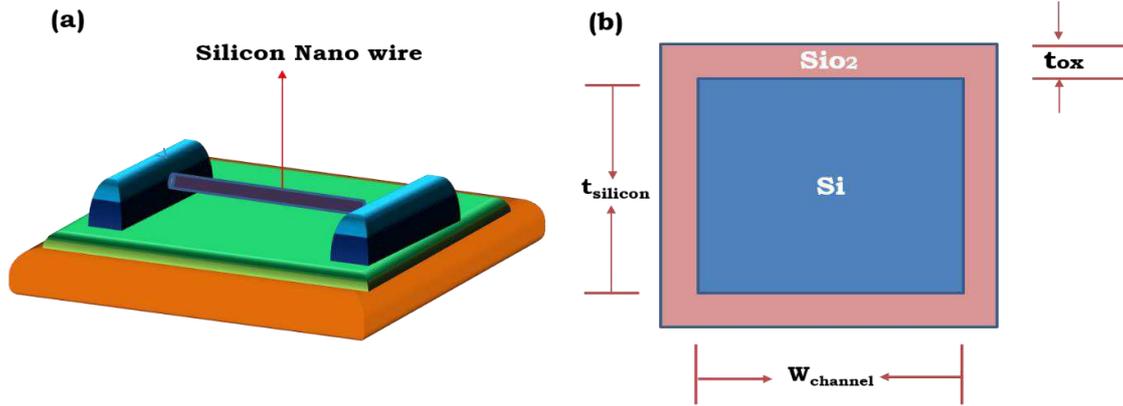


Figure 1: Schematic structures: (a) SiNW FET and (b) Cross-sectional View

The cross-sectional view of SiNW FET shown in Figure 1(b). The doped SiNW is surrounded by oxide layer with a thickness of t_{ox} . The channel width is expressed in terms of width of the oxide layer as follows.

$$\text{Total width} = \text{width of the SiNW(channel)} + 2 * \text{oxide thickness.}$$

The electrical properties of the designed SiNW FET in the absence and presence of the biomarker materials are crucial parameters to determine the overall sensing performance of the device.

2.1: SiNW FET design using COMSOL Multiphysics

A SiNW FET was designed with different device parameters. A SiNW FET with 30nm Gate length, Source and drain lengths of 40nm was designed. The design parameters of designed structure were shown in the following Table 1.

Table 1: Device parameters of SiNW FET used in the COMSOL simulations.

Device Parameter	Value
Gate Length (L_{gate})	30nm
Channel Width ($W_{channel}$)	5nm
Oxide thickness (nm)	2nm
Source Length (L_{source})	40nm
Drain Length (L_{drain})	40nm
Oxide dielectric constant ($\epsilon_{ps_{ox}}$)	3.9
Drain Voltage (V_d)	0.05 V

The SiNW FET structure was designed with semiconductor module present in COMSOL Multiphysics as shown in Figure 2. The software proficiently permits to assign physical properties of the materials to model the required structure. The investigated characteristics of the proposed structure are shown in the following sections.

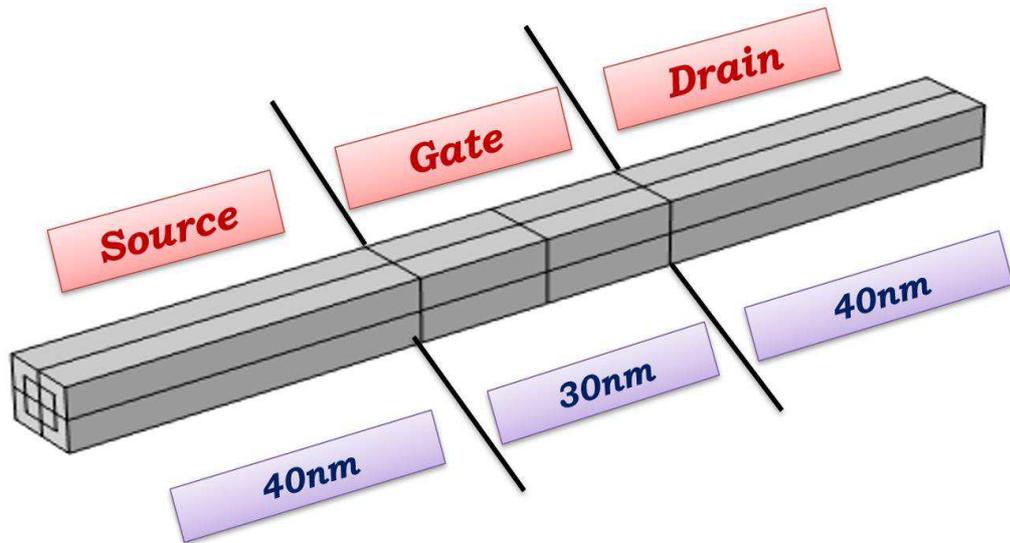


Figure 2: Designed structure of SiNW FET in COMSOL

SiNW FET of various gate lengths were designed using simulation tool. For the effective identification of characteristics, the Gate, Source and Drain lengths are prompted to 30nm, 40nm and 40nm respectively. With these fixed lengths, the determination of bio markers' presence or absence will be identified with ease. Immobilized antibodies (monoclonal Antibodies) are required to identify respective biomarkers.

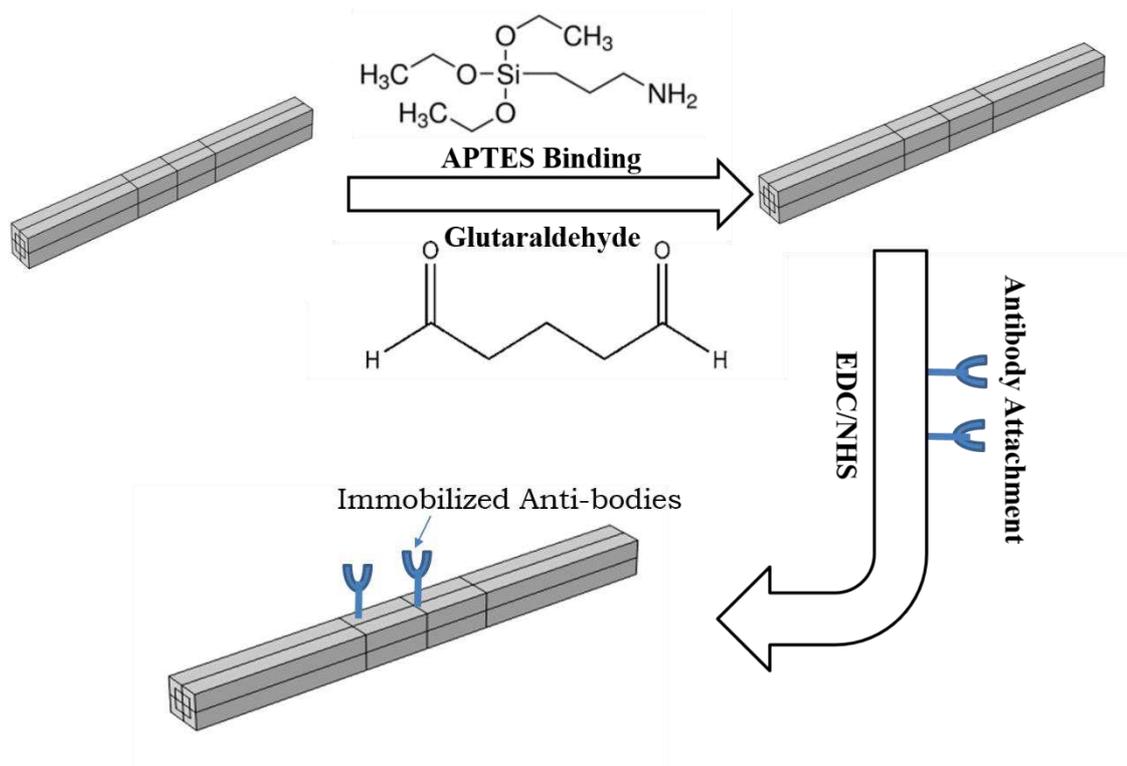


Figure 3: Procedural steps for immobilization of mAb cTnI.

As shown in the above Figure 3, A SiNW FET is equipped with mAb in order to identify the respective cTnI antigens. First SiNW FET sensor was salinized with Glutaraldehyde. Further it is synthesized with EDC (1-ethyl-3-(3-dimethylamino) propyl carbodiimide, hydrochloride and Sulfo-NHS to make mAb immobilized. A SiNW FET is a three-terminal device, comprises of a SiNW channel between two electrode terminals, source and drain.

The gate contact of the nanowire used to control the electronic response of the channel. In this section, the general behaviour of electrical characteristics of the SiNW FET device are valued in the presence of mAb and in the absence of cTnI biomarker Figure 4 (a) & (b). In the presence of antibodies and absence of cTnI biomarker, the conductance is high when compared to the bare SiNW conductance. The current is increased when mAb are attached to NW FET sensor. The conductance value of the designed structure is decreasing with the time component [14].

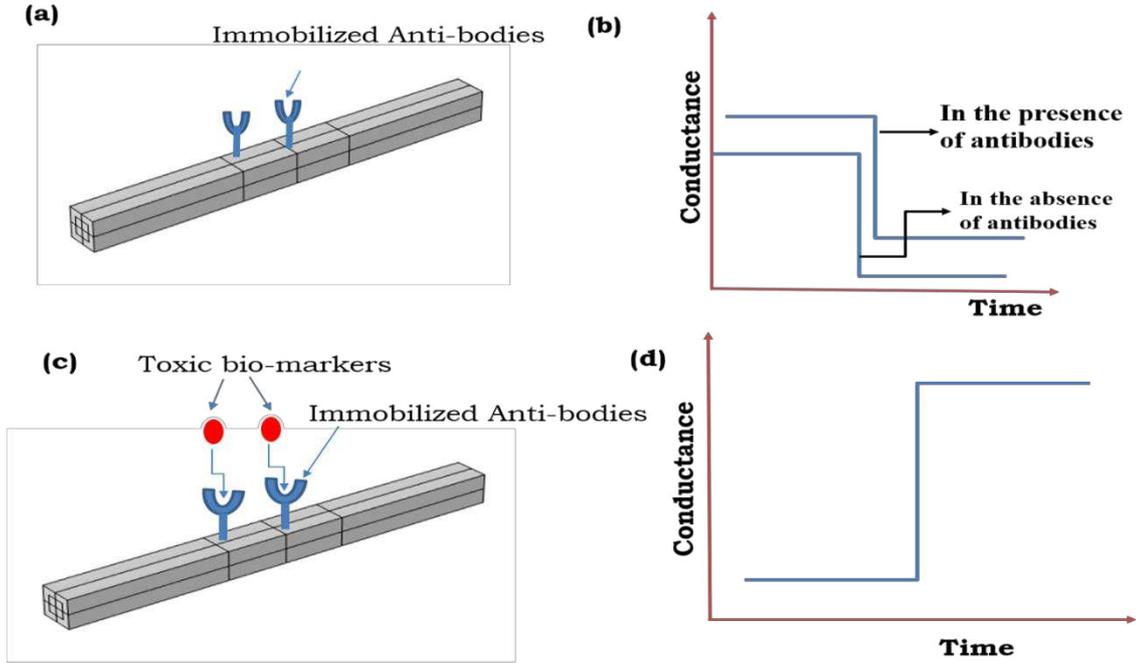


Figure 4: The designed structure with immobilized anti-bodies (a) with no cTnI bio-markers (c) with cTnI bio-markers (b) & (d) Nature of the SiNW FET sensor with and without presence of antibodies response as Conductance Vs Time.

Normally, the current of the device can be expressed as a function of different device parameters like width of the channel, length of the channel, mobility of charge carriers etc. The drain current equation is given by,

$$I_d = (W/L) * [q\mu_n n + q\mu_p p + ((\mu_n + \mu_p)/2) qn_{pud}]$$

Where μ_n and μ_p are electron and hole mobility, respectively;

$\sigma = q\mu_n n + q\mu_p p$ is the conductivity of the channel.

$((\mu_n + \mu_p)/2) qn_{pud}$ denotes that the residual charge occurs due to the spatial homogeneity.

For these analyses, the length of the channel (L_{gate} - gate terminal length) and width of the channel ($W_{channel}$ - gate width) of the nanowire FET device are considered 30nm and 5nm, correspondingly as shown in the above Figure 4 (c). A SiNW FET is equipped with mAb and exposed to respective cTnI antigens. Then the characteristics of the SiNW FET device are valued as shown in Figure 4(d). The conductance value of the designed structure is significantly increasing with the time component [14].

2.2: Analysis of SiNW FET

The particular identification of immobilized Antibodies and antigens arises at the SiNW FET biosensor gate. This can be labelled as a Chemical reaction process [15]. It can be quantified as the concentration of Antigen taking part reaction with Antibody. It is expressed as



these cTnI antigens are transported out of the solution towards the immobilized antibodies (mAbs). This can be specified as



Where $[C]_{\text{Antigen}}$ is cTnI concentration,

$[C]_{\text{Antibody}}$ is mAb cTnI concentration,

$[C]$ is the complex concentration,

$[C]_{\text{AB}}$ is the concentration of cTnI in the bulk fluid.

The modelling has been done for low fluid quantities and small-scale designs. Hence, the flow is taken as laminar as there is no turbulence and it is a steady flow [16].

$$\partial \rho / \partial t + \rho \nabla \cdot \mathbf{U} = 0$$

$$\rho [\partial \mathbf{U} / \partial t + \mathbf{U} \cdot \nabla \mathbf{U}] = -\nabla P + \mathbf{F} + \mu \Delta \mathbf{U}$$

Where \mathbf{U} - velocity, P - pressure in Pa; \mathbf{F} - body force; ρ - density and μ - dynamic viscosity.

By considering diffusion of Antigens is expressed by Fick's second law, which can be expressed as

$$\frac{\partial C}{\partial t} = \chi \frac{\partial^2 C}{\partial x^2}$$

In which the term $\partial C / \partial t$ represents accumulation and expressed in $\text{cm}^{-3} \text{s}^{-1}$,

χ is the diffusivity in cm^2/s .

The above equations are solved based on discretization the sensor area in small volume elements. We used a user defined a mesh consisted of tetrahedral or mapped elements with a mesh refinement with electrical potential structure of SiNW FET as shown in in Figure 5. The number of iterations were given as 4. The obtained variations in the mesh for different element numbers are encouragingly similar. All 3D simulations were performed with a total elements number this 3D simulation is 164920.

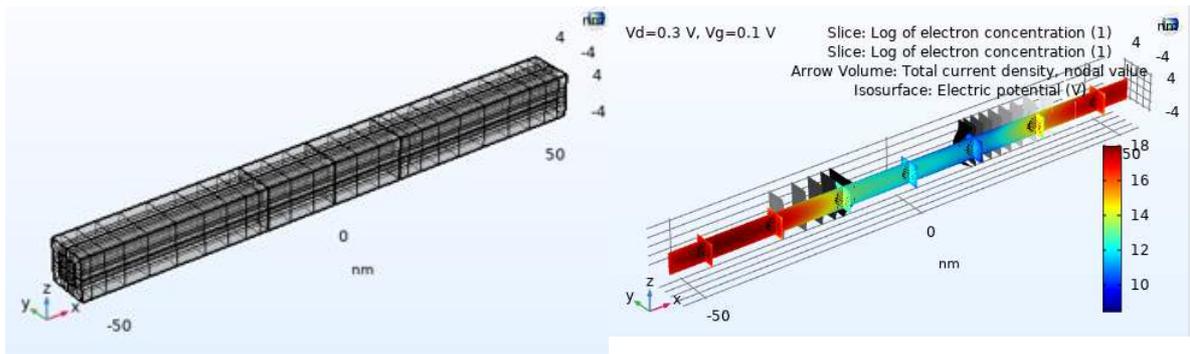


Figure 5: Meshing and electrical potential structure of SiNW FET sensor.

The designed sensor is responded to monoclonal Antibodies concentration of 10ug/mL. Then it responded to cTnI concentrations starting from 100 pg/mL and it is further diluted with PBS (Phosphate-buffered saline) to reach a concentration of 2pg/mL. The sensor is responded up to 2pg/mL. The current value obtained at 1pg/mL is almost equal to the current obtained at mAb response. The detailed results discussed in the next section.

3. Results and discussion

The length of the channel (L_{gate} -gate terminal length) and width of the channel ($W_{\text{channel-gate}}$ width) of the nanowire FET device are considered 30nm and 5nm, correspondingly. A pure Silicon with no doping concentration is used as nanowire. When the source is connected to ground, the drain current (I_d) is measured by varying the gate voltage (V_g) from 0 to 1 V at a constant drain voltage (V_d) 0.2 V, 0.3 V and 0.4 V. In the drain characteristics, the drain current (I_d) is calculated by sweeping drain voltage from 0 to 1V at different constant voltages of gate (V_g) like 0.6V, 0.8V, and 1V. the obtained drain and transfer electrical characteristics of the simulated SiNW FET were shown in the Figure 6(a) & (b).

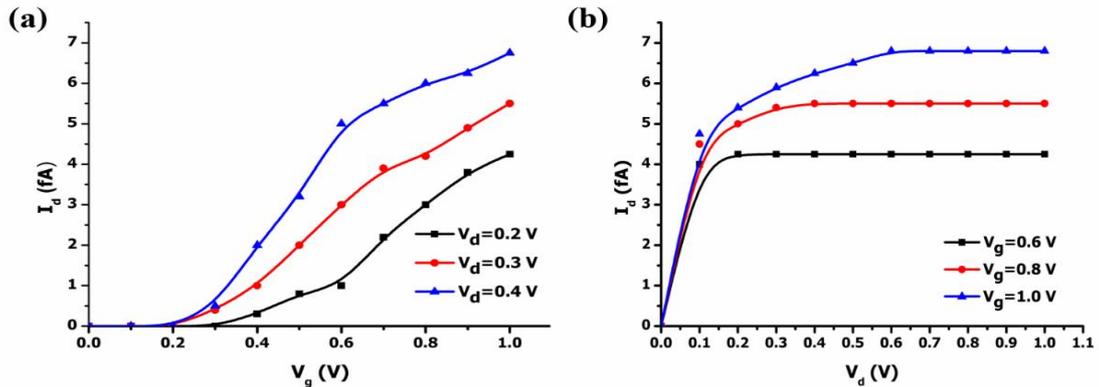


Figure 6: Electrical characteristics of the simulated SiNW FET (a) V_g - I_d (b) V_d - I_d

As shown in the above figure, the characteristics of silicon without any bio marker produces a current of the order of femto-amperes. The special behaviour of the I-V characteristics of the nanowire FET with in small range of voltages is employing the capability to identify the bio markers with detectable changes of current. Therefore, the small change in the drain current along the channel gives more insight into the I_d - V_d curve. The channel conductance is evaluated by the availability of charge carriers, which is influenced by the applied gate voltage. The conductance in return controls the drain terminal current. The carrier concentration (electron and hole) in the channel that exhibits the occurrence of inversion in the channel of the device. In this section, the SiNW FET is exposed to bio-markers with which analysed the performance characteristic changes with respect to applied voltages. SiNW FET of 30nm gate length, 40nm source and drain lengths is designed with mAb presence and it is exposed to a cTnI presence as shown in Figure 4(c). The presence of bio-markers will bring characteristic changes in the device performance in parameters like drain current, threshold voltage etc.

A SiNW FET sensor in the presence of antibodies is exposed to different cTnI concentrations. Then the source is connected to ground, the drain current (I_d) is measured by varying the drain voltage (V_d) from 0 to 1 V at different constant gate voltage (V_g) 0.6, 0.8 V and 1 V as shown in Figure 7 (a) & 7(b).

By observing the analytical characteristics, SiNW FET sensor with bio markers produces a current of the order of few micro amperes. The special behaviour of the I-V characteristics of the nanowire FET with in small range of voltages is employing the capability to identify the bio markers with detectable changes of current. Therefore, the small change in the drain current along the channel gives more insight into the I_d - V_d curve.

3.2.1. Detection of Biomarker

To perform this analysis, a SiNW FET of channel length 30nm and width of 9nm (including oxide thickness which is surrounded) and a p-type substrate is used. The doping concentration of source and drain is the order of $1E17$ is used. The drain voltage is varied in the range of 0 to 1 V, with the different concentrations of cTnI like 2 pg/mL, 5 pg/mL and 10 pg/mL. An adsorption concentration of one molecule per square nano meter of the biomarker was considered on the nanowire.

To check the sensitivity of this nanowire FET device with respect to cTnI, the drain characteristics are assessed in the presence of a cTnI and compared with a reference test in the absence of cTnI and in the presence of mAb. The designed SiNW FET is changed its drain current when there exists a mAb cTnI with respect to the design parameters. The maximum current without any biomarker is 6.5×10^{-15} amperes whereas the presence of cTnI biomarker raises the maximum drain current to 1.15×10^{-6} amperes. From the figure 7(b), the concentration drain current obtained at 1pg/mL is almost equal to that of with mAb value with which we can say that the designed sensor is having the capability to sense a minimum value of 2pg/mL of cTnI antigen which is highly recommended.

As shown in the Figure 6(a), for a bare sensor the current is the order of few femto amperes and almost equal to zero. The drain current increases when monoclonal antibodies are immobilized on the sensor. the drain current raises up to 6micro amperes. The Drain current is varied with concentration presence of cTnI biomarker. It is observed that the drain current for the SiNW FET when is not observed the biomarker is far less than that of adsorbed SiNW FET current. This behaviour of the nanowire FET is due to the effect of adsorption on the carrier mobility of the channel. An increase in drain current will be associated with the increase in mobility of the carriers and vice versa [17-18].

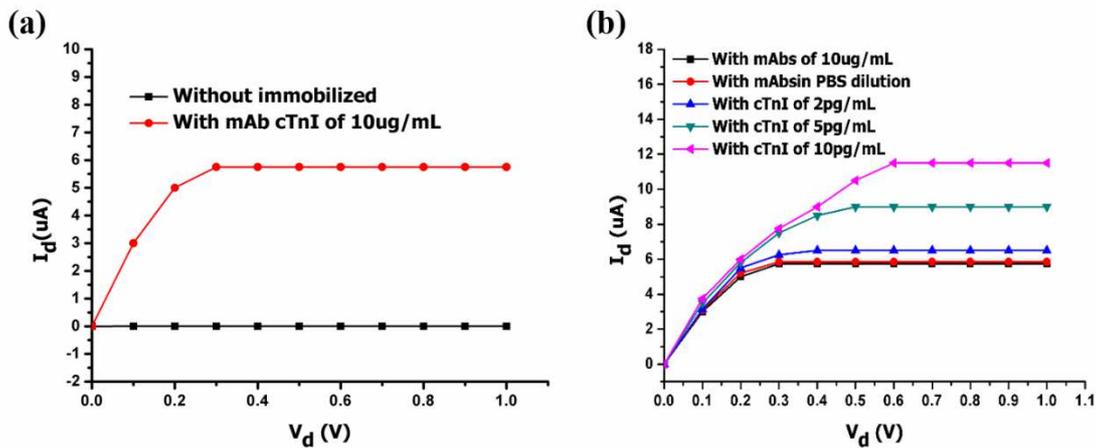


Figure 7: Analytical characteristics of SiNW FET sensor with (a) mAb (b) different concentrations of cTnI antigen

The detection of biomarker up to lower concentrations is also a big task. The designed sensor detects a lower concentration of 2pg/mL. Figure 8 shows the relation between time vs drain current. Higher the concentration of biomarkers leads to higher the conductance which leads to higher drain current. With this analysis, we can identify that the designed sensor having the capability to detect a smaller concentration from 2pg/mL to 100pg/mL when the concentration is changed at a duration of 10 minutes for each as shown in Figure 8(a-e).

Whereas the normal range of cTnI is far greater than we detected using this nanowire FET sensor. With a bare sensor i.e., with immobilized antibodies and with no antigen concentration the drain current is almost equal to the current obtained with Phosphate buffered saline (PBS).

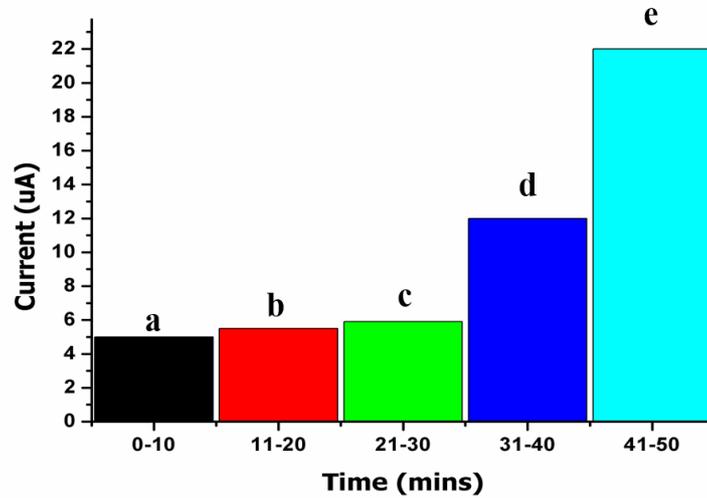


Figure 8: Detection of SiNW FET with -Impact of different concentrations of antigens on drain current (a) Bare SiNW FET (b) With PBS (c) 1pg/mL (d) 10pg/mL (e) 100pg/mL

With which we can observe that the device sensor is reactant to smaller amounts of antigen concentrations.

As shown in Figure 8(a-e), the designed sensor having a highest limit of detection in the order of 2pg/mL whereas the recent studies have a limit of detection of 2ng/mL [19] and with other types of biosensor comparison of the limit of detection for cTnI are shown in Table 2. The raise in concentration of antigen of cTnI brings raise in the drain current of the proposed SiNW FET sensor.

Table 2: Comparison of the limit of detection for cTnI biosensors.

Types	Materials	Limit of detection (ng/mL)	Ref.
FET	SnO ₂ nanowire	2	[19]
Electrochemical immunoassay	Silver enhancement	0.5	[20]
Photonic crystal biosensor	Silica and silicon	0.1	[21]
Guided-mode resonance (GMR)	GMR filter chips	0.05	[22]
Nanoelectrodes arrays	Carbon nanofiber	0.2	[23]
FET	Silicon nanowire	0.092	[24]
FET	Si nanowire	0.002	This work

4. Conclusion

In this work, the device was designed and characterized using COMSOL Multiphysics. The characteristics of the SiNW FET, which has bipolar behaviour, was observed using different characteristic measurements. These device characteristics are not only sensitive to the doping level of the silicon but also, they are sensitive to biomarkers. This investigation shows that electrical properties of the designed SiNW FET in the absence and presence of the cTnI biomarkers are largely affected the characteristics of the sensor. The device is more sensitive

to the adsorbed biomarker. The obtained I-V characteristics of the device is used to identify a Cardiac Troponin I from a lower concentration to higher concentration ranges from 2pg/mL to 100pg/mL. The designed SiNW FET sensor also has a high detection limit (~ 2pg/mL).

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Conflict of Interest

The authors declare that they have no conflict of interest.

Author contributions

M. Durga Prakash and Shaik Ahmadsaidulu: Conceptualization; M. Durga Prakash and Shaik Ahmadsaidulu: investigation; M. Durga Prakash, Shaik Ahmadsaidulu, B. Vamsi Krsihna and B V V Satyanarayana: resources; M. Durga Prakash, Shaik Ahmadsaidulu, B. Vamsi Krsihna and B V V Satyanarayana: data curation; M. Durga Prakash and Shaik Ahmadsaidulu: writing—original draft preparation; M. Durga Prakash and Shaik Ahmadsaidulu: writing—review and editing; M. Durga Prakash and Shaik Ahmadsaidulu: visualization; M. Durga Prakash: supervision;

Availability of data and material

No supplementary materials

Compliance with ethical standards

This article does not contain any studies with human or animal subjects.

Consent to participate

Additional informed consent was obtained from M. Durga Prakash identifying information is included in this article.

Consent for Publication

Author(s): Dr. M. Durga Prakash



Author's signature: M. D. Prakash ()
Date: 25-05-2021.

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Figures

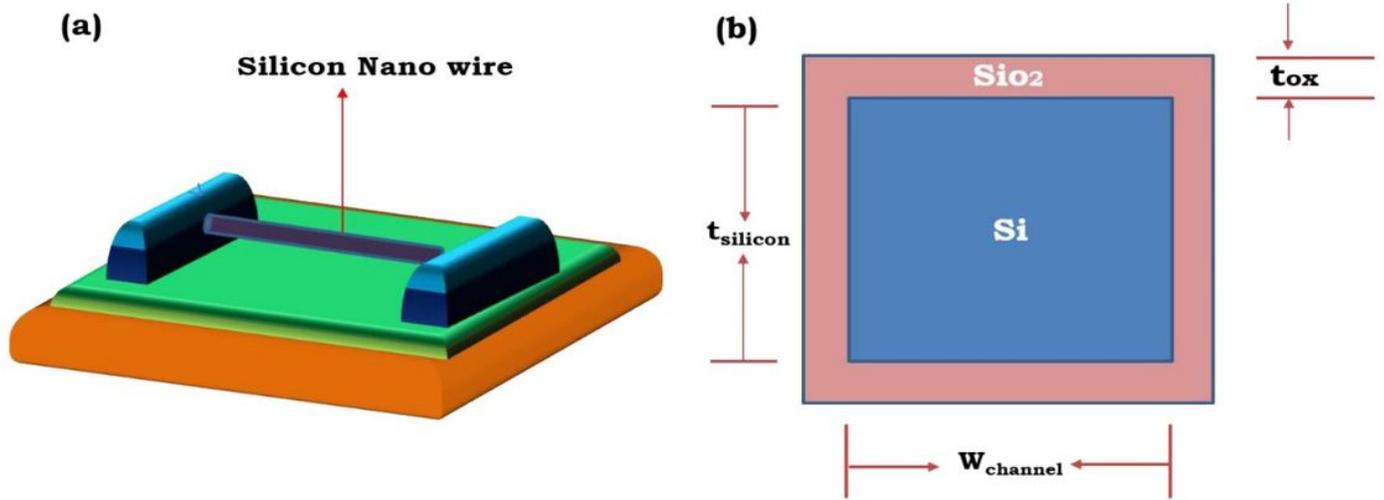


Figure 1

Schematic structures: (a) SiNW FET and (b) Cross-sectional View

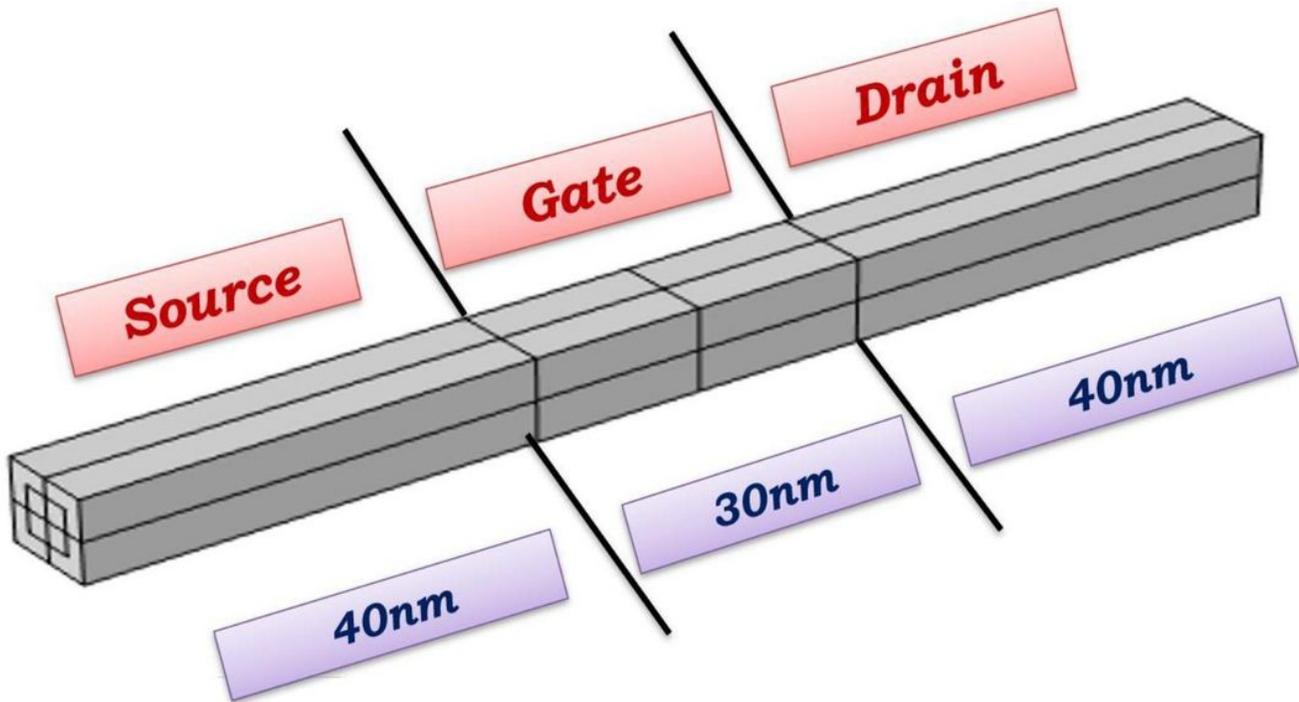


Figure 2

Designed structure of SiNW FET in COMSOL

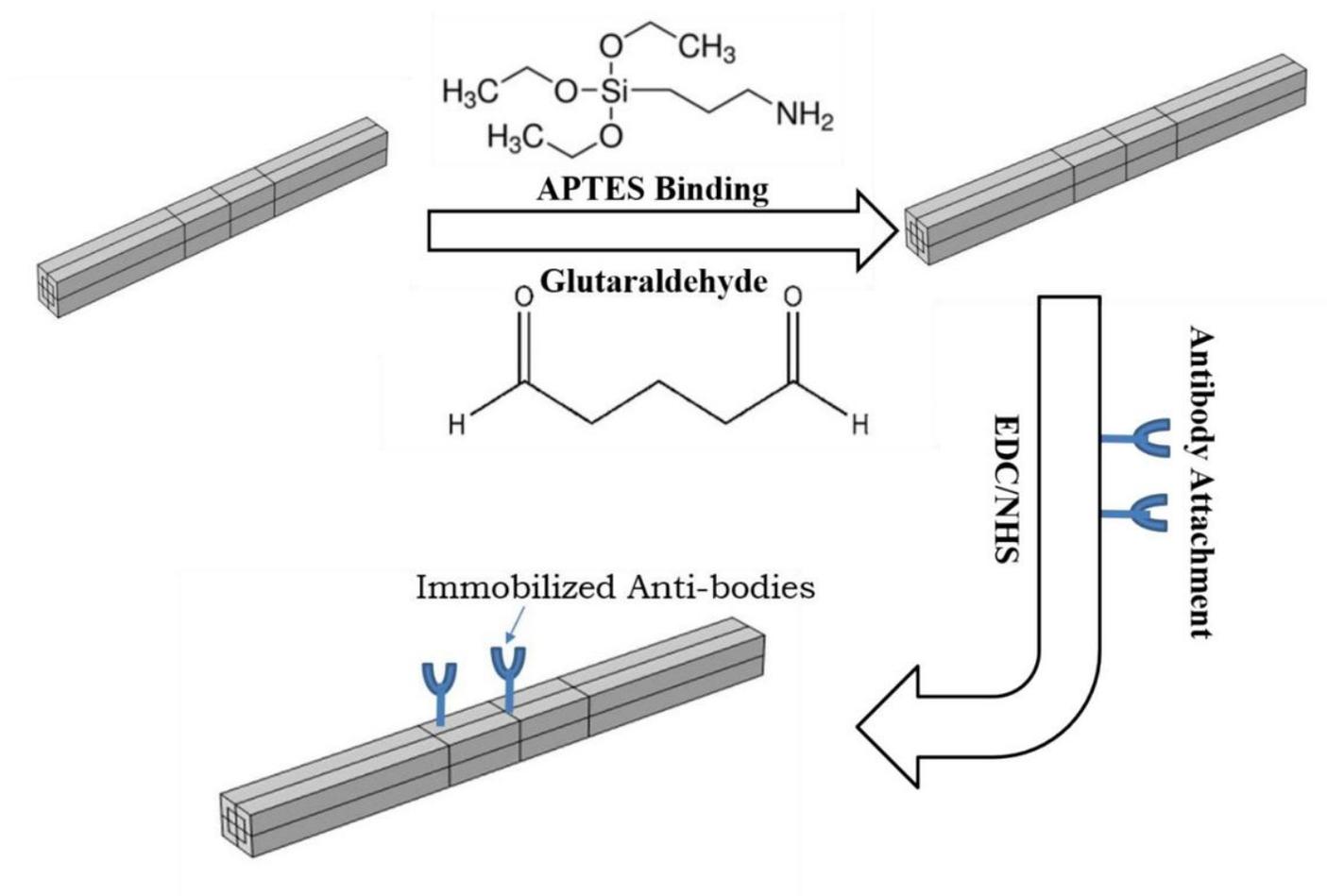


Figure 3

Procedural steps for immobilization of mAb cTnl.

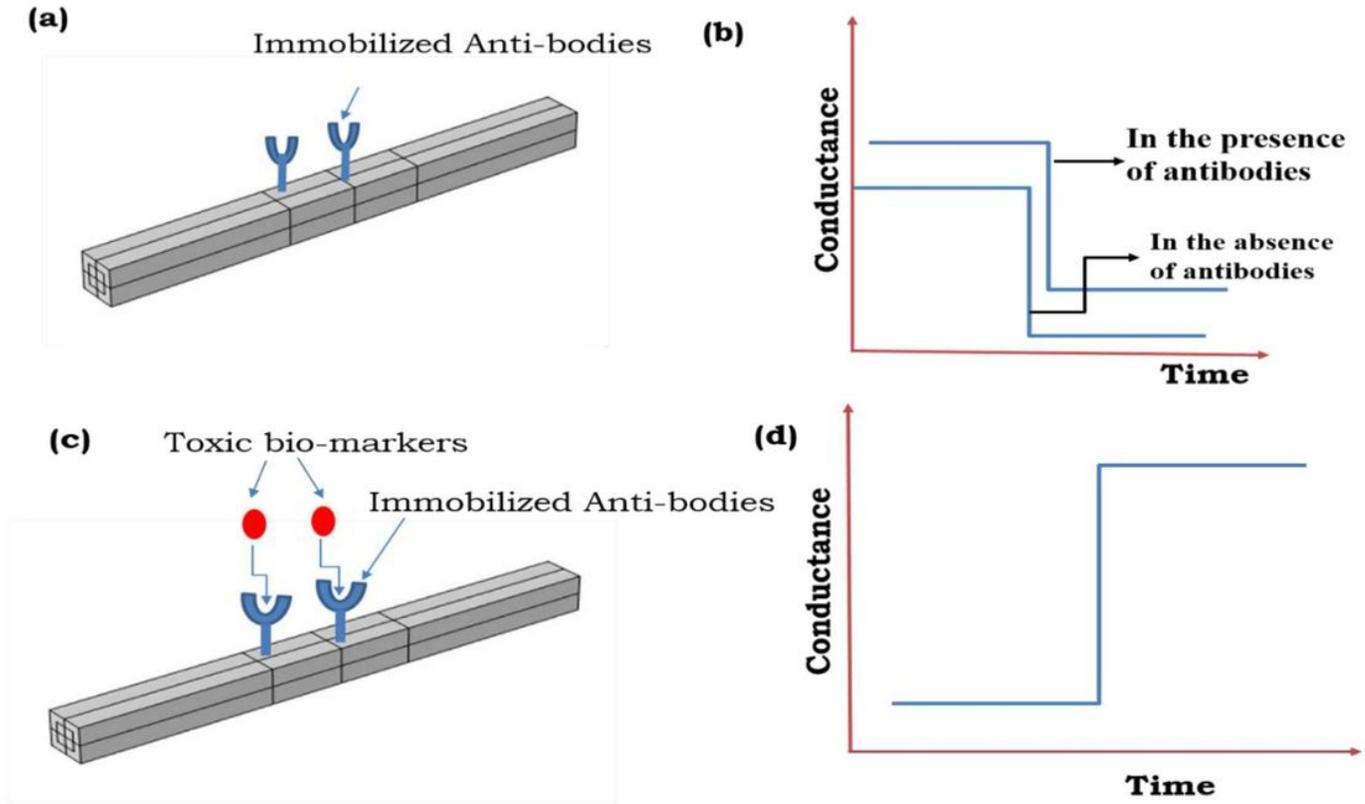


Figure 4

The designed structure with immobilized anti-bodies (a) with no cTnI bio-markers (c) with cTnI bio-markers (b) & (d) Nature of the SiNW FET sensor with and without presence of antibodies response as Conductance Vs Time.

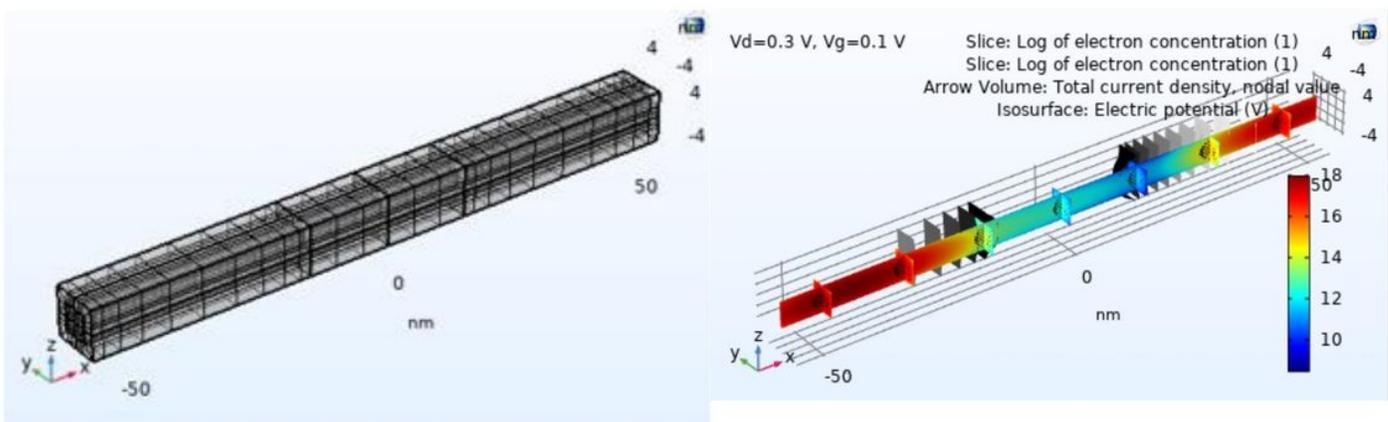


Figure 5

Meshing and electrical potential structure of SiNW FET sensor.

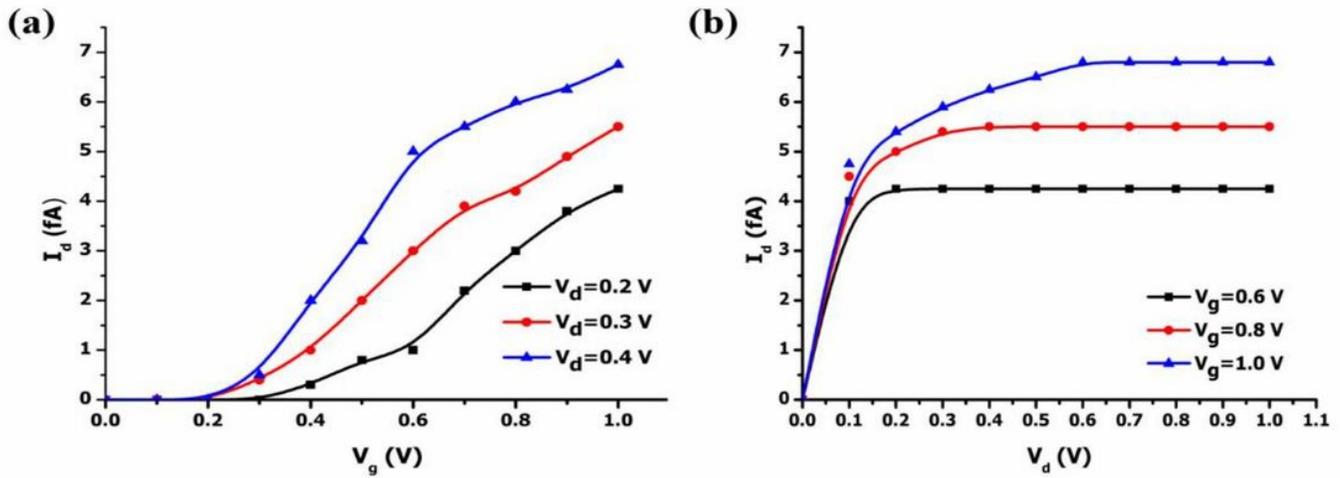


Figure 6

Electrical characteristics of the simulated SiNW FET (a) V_g - I_d (b) V_d - I_d

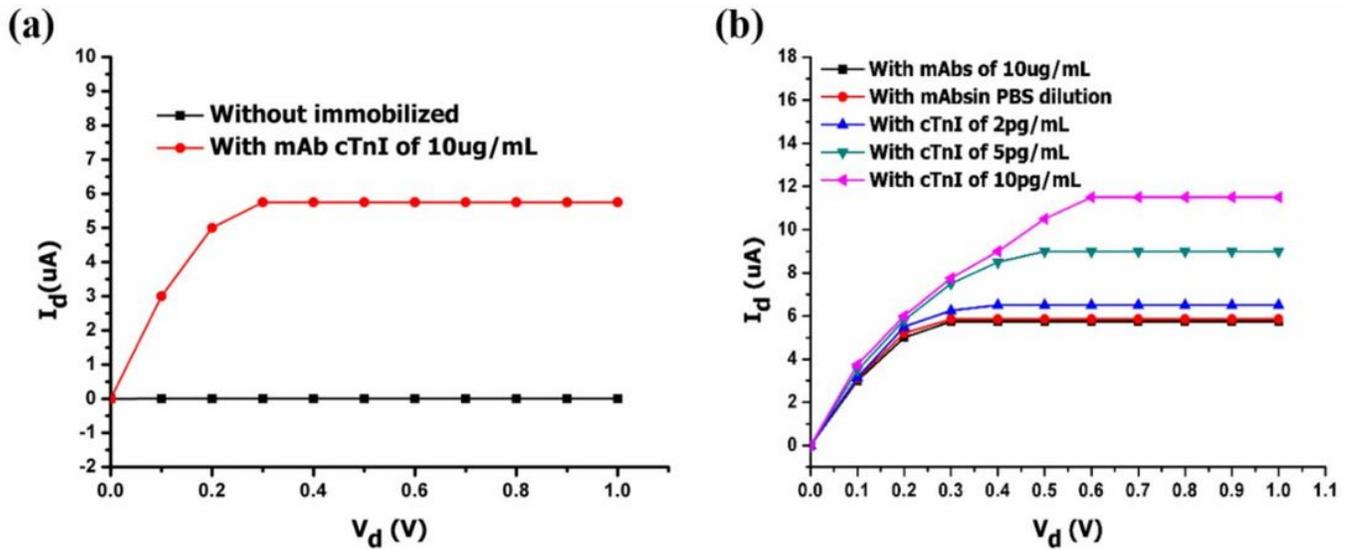


Figure 7

Analytical characteristics of SiNW FET sensor with (a) mAb (b) different concentrations of cTnI antigen

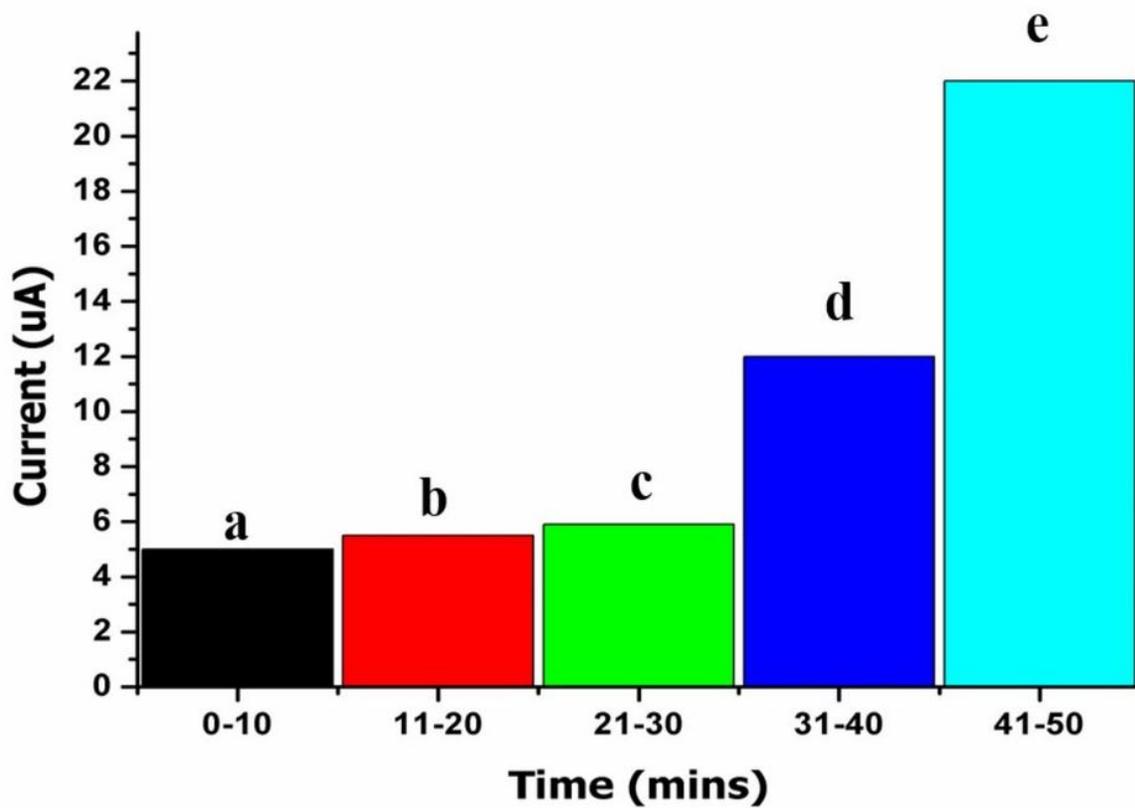


Figure 8

Detection of SiNW FET with -Impact of different concentrations of antigens on drain current (a) Bare SiNW FET (b) With PBS (c) 1pg/mL (d) 10pg/mL (e) 100pg/mL