An Investigation of the Distribution of Electric Potential and Space Charge in a Silicon Nanowire

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The distribution of electric potential and space charge in a silicon nanowire has been investigated. First, a model of the nanowire is generated taking into consideration the geometry and physics of the nanowire. The physics of the nanowire was modelled by a set of partial differential equations (PDEs) which were solved using the finite element method (FEM). Comprehensive simulation experiments were performed on the model in order to compute the distribution of potential and space charge. We also determined, through simulation, how the characteristic of the nanowire is affected by its dimensions. The characterization of the resulting nanowire, calculated by COMSOL Multiphysics, shows different dimensions and their effect on space charge and electrical potential

Key words: Nanowire; COMSOL; Biosensor; Space Charge Method; Nanotechnology.

1. Introduction

Nowadays, computer aided design (CAD) and simulation has become part of research and development in the fields of science and engineering. Numerical analysis of components, in particular, is important when developing new products or optimizing designs. The current study uses numerical simulations to investigate biomolecular interactions with semiconducting silicon nanowire surfaces at multiple levels of resolution.

Recently, enormous progress has been made in different areas related to silicon nanowires. Among them, very-large-scale-integration technology has made it possible to fabricate small dimension nanowires by saving time and money. Another area is the biomedical application of nanowires, which has recently attracted considerable attention of relevant research communities [1, 2]. A research trend is inclining towards detection of biological macromolecules using silicon nanowires, where the basic working principle is to detect the change in conductance due to the presence of partial charge in the macromolecule. In these biomolecule detection systems, the partial charge of the macromolecules on the surface of the nanowire can modulate the carrier distribution over the entire conduction pathways. This results in an increased sensitivity of the nanowire based detector [1, 3].

Currently, the COMSOL Multiphysics package [4] is a powerful interactive environment for modelling and simulation of various kinds of scientific and engineering problems based on partial differential equations (PDEs). It facilitates the development of new models associated with problems in science and engineering and allows the researcher to add physics to the model with appropriate boundary conditions [3, 5]. The researcher can specify a system of equations representing the system's behaviour. COMSOL provides necessary tools to solve the equations using finite element methods (FEMs). In the current context, COMSOL will be used to model the electrostatic behaviour of nanowires in the presence of a DNA molecule in the proximity of a fictionalization layer around the nanowire [3, 4, 6].

In this study, the model nanowire is a nanostructure with the diameter of the order of a nanometer (10^{-9} m). Alternatively, nanowires can be defined as structures that have a thickness or diameter constrained to tens of nanometers or less and an unconstrained length. At these scales, quantum mechanical effects are important which coined the term 'quantum wires'.

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Many different types of nanowires exist, including metallic (e. g., nickel), semiconductor, and insulating (e. g., silicon dioxide). Molecular nanowires are composed of repeating molecular units either organic (e. g., DNA) or inorganic [6 – 8].

The organization of the paper is as follows. The next section describes a general overview of the numerical simulation using COMSOL Multiphysics, then, in Section 3, results and discussion are presented, and finally, in Section 4, a conclusion is given.

2. Modelling and Simulation

In this section, we build a model of a nanowire and discuss about adding physics and driving equations to that model.

2.1. Geometry

The first step is to generate the model geometry of the silicon nanowire. In this model, we used three-dimensional (3D) general forms of COMSOL PDE modes that are suitable for simulating the nanowire within COMSOL Multiphysics. Two geometries were considered in this investigation. In the first geometry (Fig. 1) the 3D geometry of the silicon substrate consists of gold electrodes on the silicon surface. The silicon nanowire consist of a hollow cylinder having a diameter of 0.5 cm with a membrane thickness d of 4 nm and a length L of 4 cm. The goal of the designed model is to gain an understanding of the physics of the device without much complexity [9, 10].

2.2. Equations and Parameter Setting

In this step, we include all parameters and relative equations to simulate the silicon nanowire. The physical parameters of the device consist of dimension and space charge, as well as various conditions such as subdomain setting, boundary conditions etc. We described material properties, sources, and PDE coefficients on the subdomains. On the subdomains it is also possible to specify initial conditions and element types. We used an electrostatic model of COMSOL Multiphysics and set variables and constant parameters such as thickness, relative permittivity, and space charge density. The electrostatic model of micro electro mechanical systems (MEMS) is the best choice to design a silicon nanowire based sensor due to its relevancy with the model electrostatics in the subdomains [8].

The associated model is based on the following system of PDEs:

$$D = \varepsilon_0 \varepsilon_\mathrm{r} E\,, \tag{1}$$

$$D = \varepsilon_0 E + \rho\,, \tag{2}$$

$$D = \varepsilon_0 \varepsilon_\mathrm{r} E + D_r\,, \tag{3}$$

$$\nabla \cdot d \varepsilon_\mathrm{r} \varepsilon_0 \nabla = d p\,. \tag{4}$$

In the above equations, ε_0 is the permittivity of a vacuum, ε_r the relative permittivity, ρ the space charge density, and d the thickness of the nanowire. The extracellular medium is a physiological saline solution with a relative permittivity ε_r and a spatial charge density of ρ $(\mathrm{C/m^3})$. Here we specify boundary and interface conditions. Figure 2 shows the designed silicon nanowire with gold electrodes fitted with electrical potential and electric shielding. By setting appropriate boundary conditions, it is possible to observe the effects of variables, such as voltage, surface charge density, thickness, and current. All boundaries of the nanowires in the PDE subdomain are included in the equations. In the electrostatic mode, two sets of boundary conditions were considered. The first one in Figure 3a uses an electric shielding of the electrodes

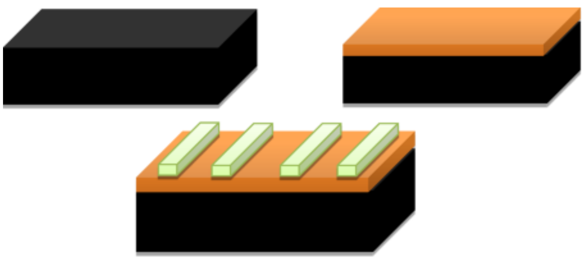


Fig. 1 (colour online). Designed model of the silicon nanowire.

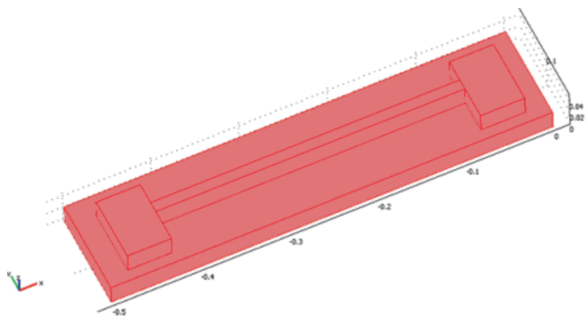


Fig. 2 (colour online). Single design of the modelled silicon nanowire using COMSOL Multiphysics.

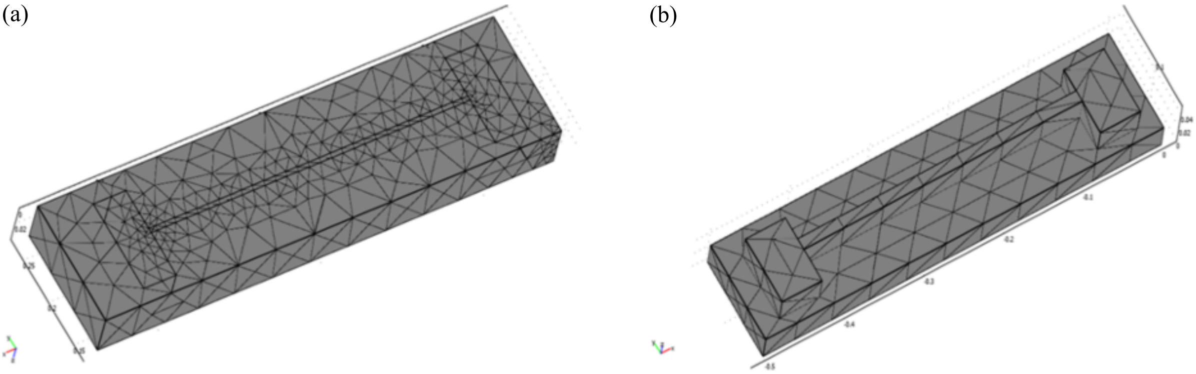


Fig. 3 (colour online). Resulting mesh of the designed model nanowire at (a) 1 V and (b) 5 V.

where the wire has an electric potential of 5 V, whereas in Figure 3b it has an electric potential of 1 V. Figures 4 and 5 display various parameters, such as thickness, relative permittity, and surface charge density, observed at 1 V and 5 V [8]. The parameters are related to the nanowire by using the following equation [8]:

The electric potential equation

$$V = V_0 \tag{5}$$

and the electric shielding equation

$$n \cdot D = \rho_s - \nabla_t \varepsilon_0 \varepsilon_r d \nabla_t V \,. \tag{6}$$

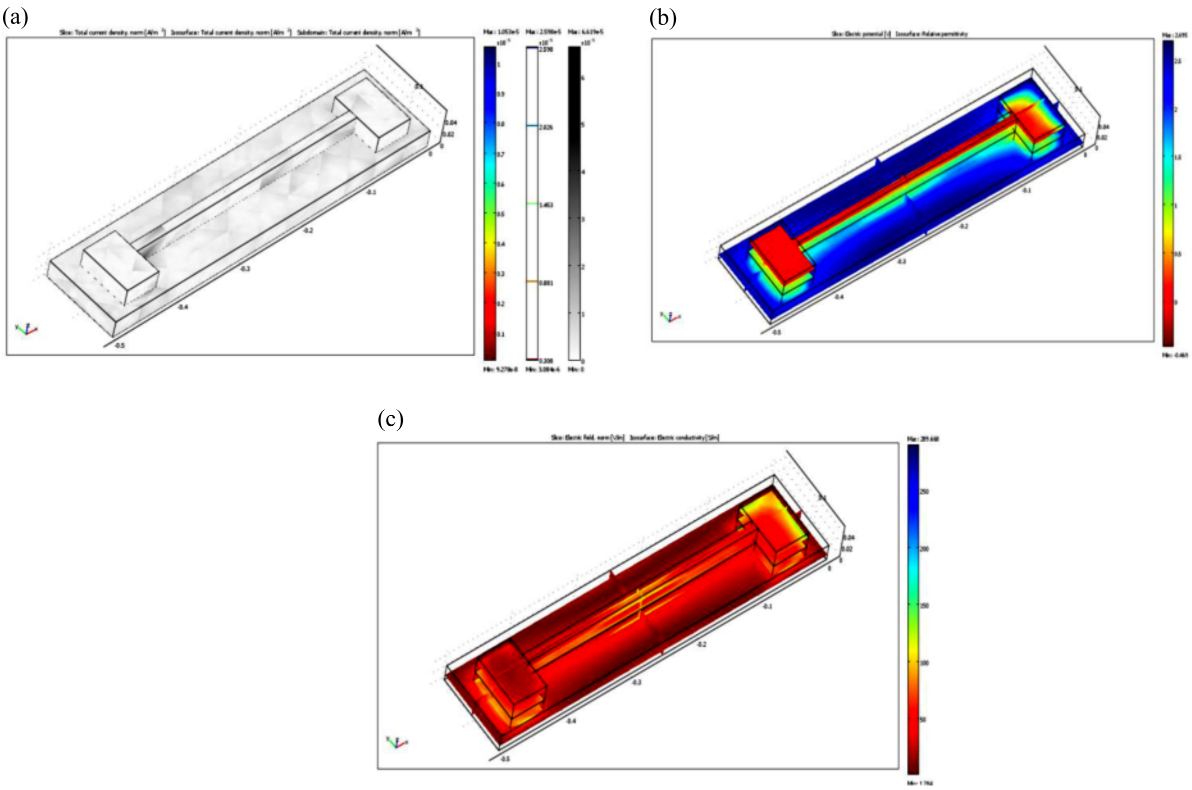


Fig. 4 (colour online). Surface charge variation as result of silicon nanowire size changes from (a) 200 nm, (b) 220 nm, and (c) 250 nm when the electrical potential is applied.

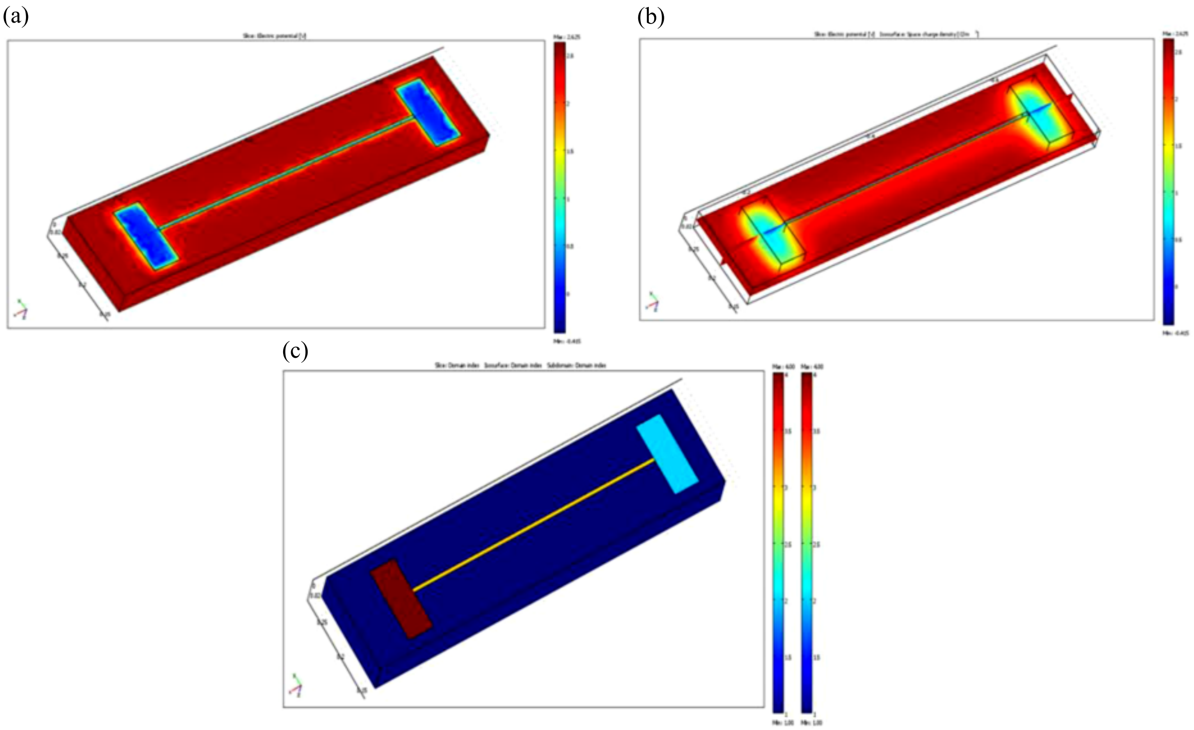


Fig. 5 (colour online). Surface charge variation as the result of silicon nanowire size changes from (a) 80 nm, (b) 90 nm, and (c) 100 nm when the electrical potential is applied.

For edge settings, we specify edge parameters and describe material properties and PDE coefficients on the edges of the silicon nanowire. On the other hand, we specify point settings and can describe properties and values for point sources and other values that apply to geometry vertices. Some application modes use scalar variables that are independent of the geometry, such as the frequency.

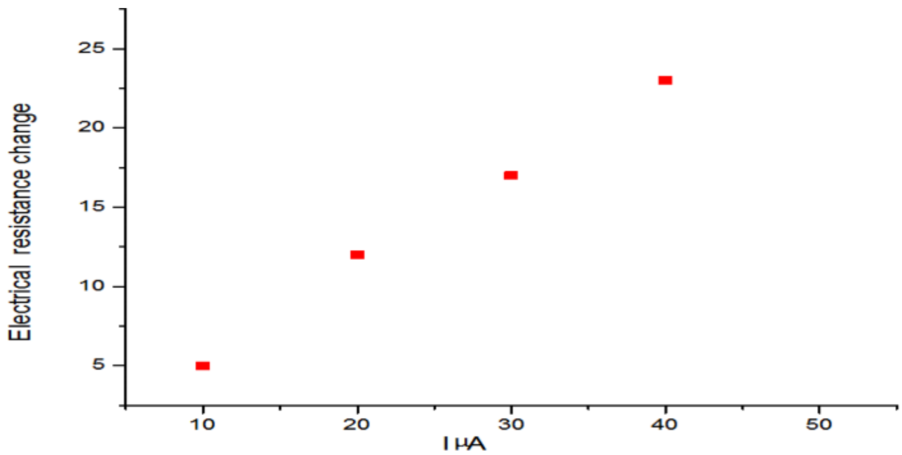


Fig. 6 (colour online). Result of the analysis for the designed nanowire of the relationship between current and electrical resistance change for a nanosize wire of 100 nm.

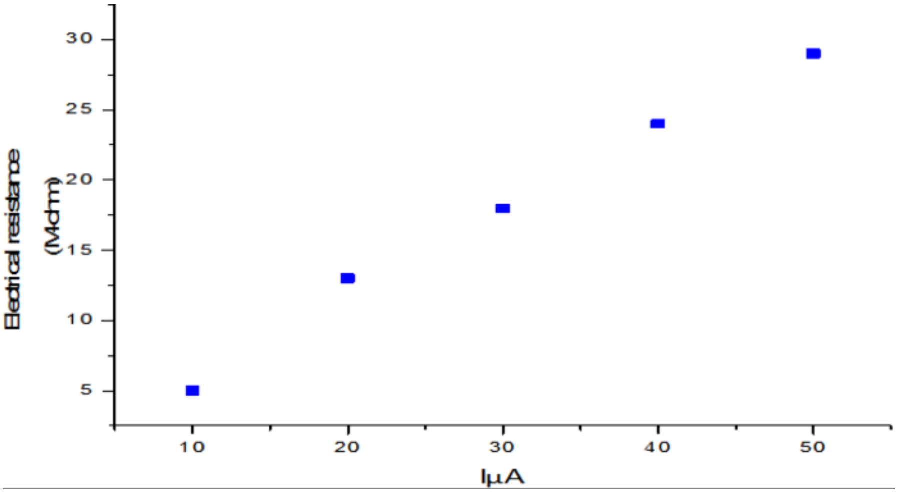


Fig. 7 (colour online). Result of the analysis for the designed nanowire of the relationship between current and electrical resistance change for a nanosize wire of 200 nm.

2.3. Mesh Generation

In this section, we have generated the finite element mesh for the model geometry. It is important to judiciously determine the element size of the mesh generation. If a fine granularity is used, the results will be more accurate but the computation will demand more computing power. On the other hand, a coarse granularity will require less computational power but of the expense of accuracy of the result. The mesh model in Figure 3 shows a nanowire design with a finer mesh around the wire and the gold electrodes than in the external domain. The number of elements used in the model is nearly 300 000 in parameters and variables of free mesh such as curvature factor, curvature off, and elements. Therefore, in this design, time is very important and a dependent solver was used to consider the temporal dynamics of the nanowires. The effect of different parameters used in the mesh model provides information about various variables of the nanowire model by using an electrostatic model.

3. Result and Discussion

The study investigated the effect on the electrical properties by varying the dimensions of the nanowire.

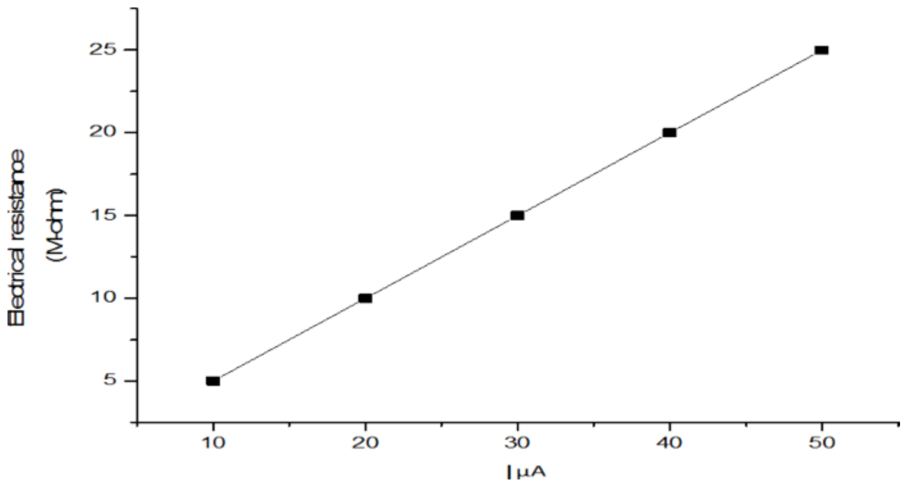


Fig. 8. Result of the analysis for the designed nanowire of the relationship between current and voltage with 350 nm.

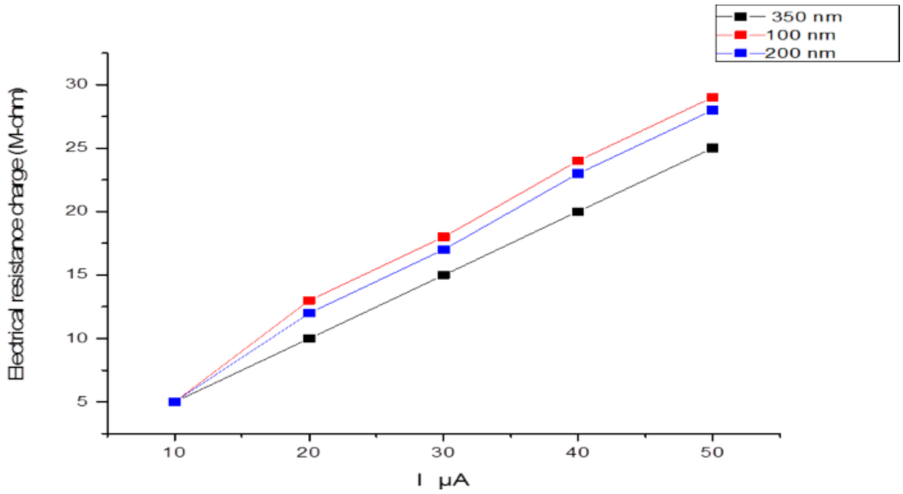


Fig. 9 (colour online). Results of the analysis for the designed nanowire of the relationship between current and electrical resistance change for different wire sizes.

At the nano level, many properties come into play. Therefore we have studied three different sizes in this work. When subjected to electrical potential, we found out that the relationship between the dimensions and the field effect transistor where controlled by the electrical potential, the current flowing through the device, and the gate voltage. Figure 4a shows the result of the simulation where the two electrodes are at the same potential with low voltage, and the wire indicates a high potential with maximum electron flow. On the other hand, the permittivities for the two materials were different because the wire consists of silicon and the electrodes were made up of gold in which gold indicates low permittivity because the electronic grain is bigger than in silicon. The simulations of the electronic behaviour of the nanowire consist of self-consistent calculations using (1) – (5) together with a modified 3D electrostatic equation that accounts for all aspects related to the lateral and vertical scaling of nanowire devices. In addition to these simulations, we observed in Figure 4b the behaviour of the silicon wire due to dimension and the degree of potential subjected on it.

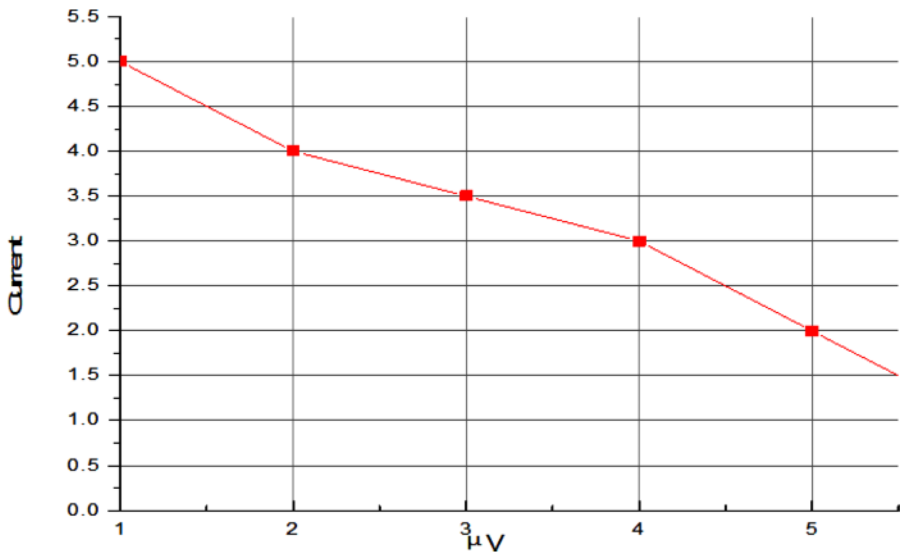
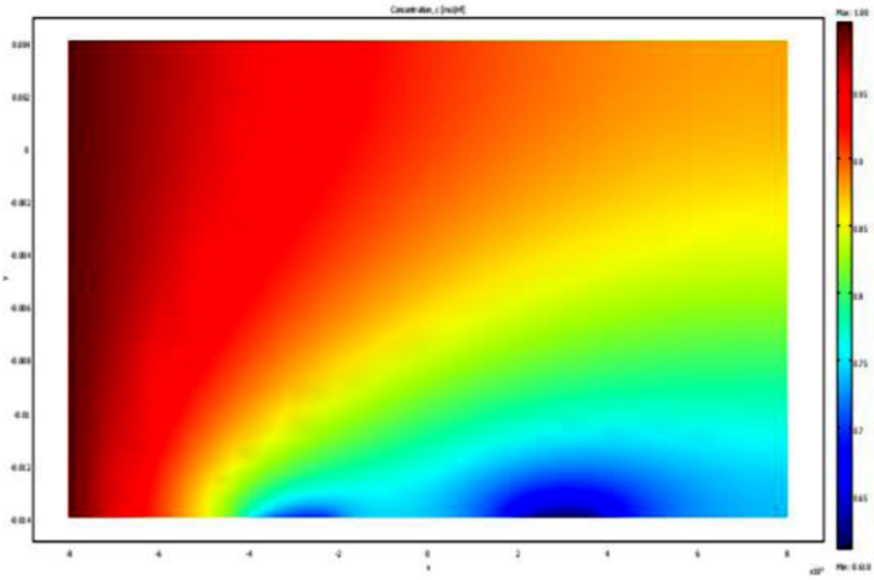


Fig. 10 (colour online). Result of the analysis for the designed nanowire of the relationship between current and voltage.

In this case, we identified the wire with high conductivity displayed in four colours, and a different colour can be seen for the gold electrode. The effect of dimensional variation is one of the most important conditions in the performance of nanowires since the radial width of silicon nanowires used for biomolecule detection is between 100 – 300 nm, what is needed for a proper interaction in the active domain. Here we use a partial

(a)



(b)

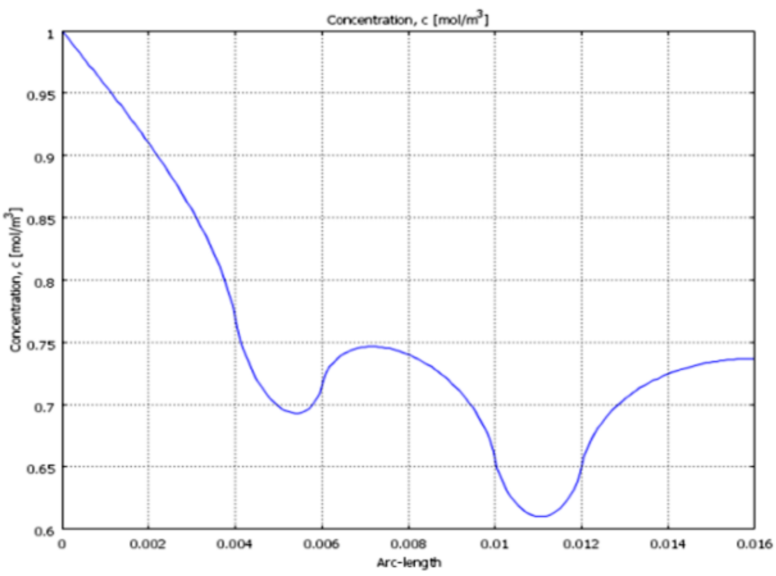


Fig. 11 (colour online). (a) Graphical result of the simulation for space charge density, (b) graphical result for the relationship between concentration and charge distribution.

electronic diffusive approach to model the conductance change due to the variation in width of the nanowire when the reaction occurred on its surface.

In the simulation result of the silicon nanowire surface, we are going to discuss the dimensions with respect to resistance and the effect of different dimensions of the nanowire surface on resistance and current characteristics. We related the resistance, length, and width of the nanowire surface by using following equations:

$$R = \alpha \frac{L}{A}, \tag{7}$$

$$R = \rho \frac{L}{A}. \tag{8}$$

In this case, the different dimensions of the nanowire surface show an effect on the resistance of the wires. It was notified that by changing the area of nanowire surface the resistance increases and the current decreases. On the other hand, the effect of width and height were related to the area by using the equation

$$R = \rho \frac{L}{XXW}, \tag{9}$$

where W is the width of the nanowire and X is the radial height. Figures 4 and 5 show the result of the designed and simulated silicon nanowire surface and the gold electrode on the silicon substrate. These figures display the effect of different dimensions on the current flow and show the structural simulation of the 3D nanowire, which is done by considering 3D electrostatic studies of finite element FEM COMSOL Multiphysics 3.5. The result indicated a variation of parameters with the variation of wire sizes. Figure 4 shows the surface charge produced by a wire of 200 nm with increasing electrical potential. Its size is not yet small enough to support the surface to volume ratio, therefore the electrical field created as a result of the electrical potential does not show enough strength. This can be seen in Figure 4 where only one out of three designs shows a relatively high potential. However, Figure 5 shows the opposite effect where two out of three designs show high potentials. This might be because of the smaller wire size of 100 nm.

One can see in Figure 4a that the surface charge density of wire and substrate are similar, moreover, the electrical potential of wire substrate and electrode have the same colour. The blue colour indicates the complete transformation of the potential on the wire area. The electric field of the modelled nanowire shows the whole potential inside the wire were the same electrical potential (same colour) is reached. This does also indicate that the current density is higher (see colour bar).

The effect of different dimensions of nanowire and electrode are displayed in Figure 5. We can see a different conductivity due to the different dimensions of the second model. Moreover, the result indicates that the mass transport is mainly responsible for the obtained wire response. It is also notable that, at a lower flow rate, a significant higher concentration of the bound complex charge density is obtained. The result demonstrates that the onset kinetics of the observed wire cannot be used to determine the intrinsic binding kinetics. It also suggests that the low response can result in a higher wire response signal so as to generate a higher signal.

Figures 6, 7, and 8 show separate curves for resistance/current response. Figure 6 reveals the current response of the 100 nm wire, and this device produced highest currents as well as the electrical resistivity. It is well known fact that, when the wire size becomes smaller, it affects electrical properties such as resistance and conductivity, mainly caused by a shrinking of the mean distance between two atoms, making it too difficult for the charge to flow freely. But due to surface phenomena, nano devices respond differently because of the surface to volume influence, what is further confirmed in Figure 7 and Figure 8. In these figures both curves show a lower resistance as a result of the bigger sizes ot the wires compared to Figure 6. All three results explained above are combined in Figure 9.

Figure 9, showing the result of the analysis of the designed and simulated silicon nanowires, is explained with the help of silicon nanowire surface properties like electrical resistance and current. Here, the thicknesses of 100, 200, and 350 nm are compared in the same graph. It is clearly seen that the width of 100 nm has higher total displacement values among other thickness values which show better sensitivity. The current gets smaller as the resistance increases and then suddenly, after a particular thickness, the voltage becomes constant. This shows that the voltage is more concentrated on the surface.

The graphics below show the result of each simulation, the relationship between electrical resistance and current (Figs. 5 – 8), and Figure 10 where the relationship between current and voltage is plotted. The voltage gets decreased as the thickness increases and then suddenly, after a particular thickness, the voltage becomes constant. This shows that the voltage is more concentrated on the surface. As we have seen in Figure 5, the 100 nm design give the desired results and this mainly is confirmed in Figure 10 and its role of the space charge effect in the I–V behaviour of an nanowire. The result confirms that the space charge effect is one of the possible factors responsible for the nonlinearity of the Fowler–Nordheim (FN) plots of an nanowire at high fields. Furthermore, one can see that the calculation reveals that the threshold field is related to the nanowire work function in an almost linear manner. On the other hand, Figure 11b shows the graphic result of the relationship between concentration and charge distribution. There is a non-negligible potential inside the silicon nanowire due to space charge at the interface between the surface of the nanowire and the electrode.

4. Conclusion

We simulated different 3D models of a silicon nanowire using electrostatic equations to quantitatively validate the existing experimental data for electrical potential and space charge distribution. The present model is a first step in nanowire–electrode coupling with a detailed electro-chemical model of nanowires. It is observed that the diameter and length of the wire affects the charge distribution. A detailed study of these effects upon variations can be performed. The parameters of electrostatic equations effect the different phases of wire dimension, its initiation and distribution.

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