

Silicon Nanowire Geometry: Investigation of Interaction Site Potential in Semiconductor-DNA Interaction

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Abstract: COMSOL Multiphysics Simulation is one of most important software package in engineering material simulation and science related design, semiconductor based nanowire have become one of critical device in bio sensing, thus simulations of this device become not only necessary to understand the nanostructures materials behaviour but also highly necessary to understand the potential parameter that can contribute to its capabilities in interacting with other different material since at the atomic level, the prediction of ion behaviour cannot be concluded using only the absolute charge. Hence, this paper presents an investigation of interaction site potential in semiconductor-DNA interaction for biomedical application

Key words: Silicon nanowire, nanotechnology, nanomaterial, piezoelectric, COMOSL Multiphysics

INTRODUCTION

In nanotechnology today, the computer simulation has become an essential part of nanotechnology and science and engineering (Anthony J. O'Lenick, Jr., 1999). Nowadays, one important aspect of nanostructures and engineering is the understanding the physical science and behaviour of a model or device can be easily captured by COMSOL simulation (Hashim, U., 2012). Digital analysis of components, in particular, is important when developing new products or optimizing designs when apply the new method in Digital analysis of components it is very significant when new yields or optimizing designs is required however, to a greater aspect simulation play a major role (Tijjani Adam, 2012). The aim of this work is to give an introduction to finite element method (FEM) software for design model nanowire, where the capability of models is explored using some examples of biomedical applications which FEM can be used for. The exercises will be performed using the commercial software COMSOL Multiphysics. There are two different exercises, the second one divided into two parts, and there are specific tasks associated with each exercise (Johannes Johansson, 2008; Th. S. Dhahi, 2012).

The chemistry semiconductor element such Si play a great role in semiconductor industry and silicon is the 14th element in the periodic table. Although it does not occur naturally free form, in its combined form it accounts for about 22-25% of the earth's crust. Silicone compounds are unique materials both in terms of the chemistry and in their wide range of useful applications. Also Silicon in combination with organic compounds provides unique properties that function over a wide temperature and mechanical strength, making the silicone products produced with this element less temperature sensitive than most organic surfactants and withstand various applications. These properties can be attributed to the strength, flexibility and ease of handling due to the Si-O bond, its partial ionic character and the low interactive forces between the non-polar methyl groups, properties that are directly related to the comparatively long Si-O and Si-C bonds structure. The length of the Si-O and Si-C bonds also allows an unusual freedom of rotation, which enables the molecules to adopt the lowest energy configuration at interfaces, providing a surface tension that is substantially lower than the organic polymers. There various ways to obtained and most common one silicon is obtained by the thermal reduction of quartz (SiO₂) with carbon. The reaction is 'melted at high temperatures and however is commonly carried out where there is abundant inexpensive power. The reaction is as explained below, the purity of the silicone is generally at least 88-99% pure. Moreover, certain trace contaminants must also be controlled to obtain a material that is suitable for the preparation of silicone compounds. Since the silicon so produced is a solid metallic material, it is crushed into powder having a particle size of between 100 and 350 nm for reaction in the Rochow process. In other hand, this process is named after Eugene G. Rochow, the father of silicone chemistry¹. Due of the complicated process technology, and high capital requirements to construct plants suitable to practice the chemistry, few companies actually carry out the Rochow process. Due the silicon is crushed prior to reaction in a fluidized bed, the companies practicing this technology are referred to as "silicon crushers". Because this is an elite group on companies, being referred to as one of the silicon crushers is considered an honor in the silicone world.

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In this paper we presented the effect of the design nanowire and gold as electrodes on the conductance of the nanowire through finite element calculations for interaction DNA application. The conductance, in turn, dictates the sensitivity of the nanowire biosensor for biomedical applications. The bio-sensor under investigation consisted of a silicon nanowire surrounded by an electrode layer.

Design Nanowire:

Geometry and Physics Setting:

In this design used two and three dimensional general form of COMSOL PDE modes used to simulate the NW-Si using Multiphysics ® 3.5a. The Original geometry of NW silicon is a hollow cylinder of 0.9 μm diameter with a Width of 200nm and a length of 4 μm (Koch, C., 1999) due to numerical limitations, such as first simulation approach, a tubular cylinder with a diameter of 25 μm , a length of 135 μm is assumed and a membrane thickness of 60 nm. Also it is supposed that the numerical problems could be avoided if the code would allow for a scaling factor for the geometry input. Figure 2 shows effected geometry single wire design 2D and 3D of NW (Koch, C., 1999).

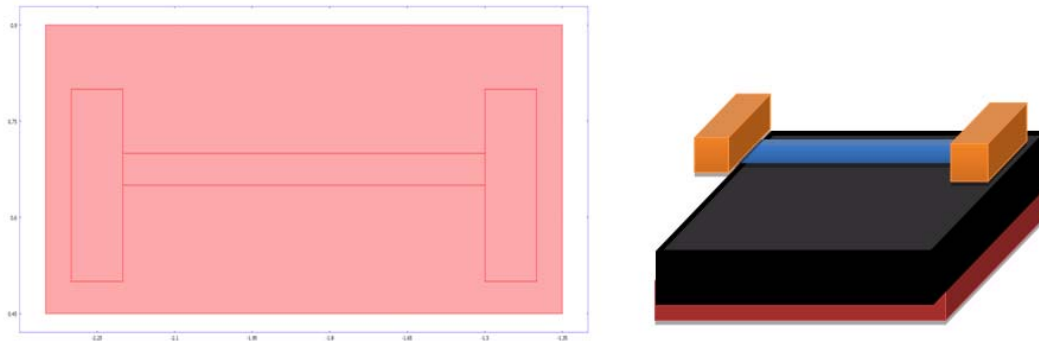


Fig. 1a: Showing design silicon nanowire of COMSOL Multiphysics, b) model design silicon nanowire and electrode.

In other hand, Boundary Conditions are the potential distribution in the extracellular medium, which is described by the piezoelectric form of the equations, is solved using the piezoelectric. The nonlinear differential equations describing the membrane behavior are coupled with the FEM solution using COMSOL Multiphysics® 3.5a. Coupling is achieved by setting the (BC) as given below. All boundaries of the cuboids axon in the PDE subdomain are taken as Neumann BCs; the normal component of the electric potential is zero. The figure below is a schematic diagram of the active boundary conditions in PDE mode. In the subdomain Setting is one mode is used in the design nanowire simulation, of wire silicon. The wire is considered as a subdomain with the dependent parameters variables. This is to facilitate the simulation to observe a detailed initiation and propagation of wire in a specified region. The external medium is considered using the dependent variable V in the piezoelectric subdomain of the PDE mode solves (Gouthami, N., 2011).

Result Simulation:

From figure 2(a,b), we design and simulated a 2D and 3D model of nanowire silicon using the piezoelectric equations to quantitatively validate the existing experimental data by using COMSOL Multiphysics, design nanowire ,electrode gold and substrate for organic applications such as DNA interaction. It is observed that the diameter and length of the axon affects the propagation velocity. A detailed study of these effects upon variations can be performed. Based on the model, parametric studies will be carried out in future for specific dimensions and Properties of the wire (Yipei Wang, 2012).

Depicts the wire and electrode obtained from the simulation. Where the two electrodes are the same potential with low voltage however, the wires indicated high potential all four wires were at the same potential with maximum electron flow. they permittivity for two material can be seen differently because wire is use silicon as material and gold for electrode but the gold indicated low permittivity because electronic grain is bigger than silicon. Simulations of the electronic behaviour of Nano wire consist of self-consistent. In addition to these simulations, infig 2 we see behaviour of silicon wire due to dimension and the degree of potential subjected it, in this case we identified the wire with high piezoelectric through four colours, moreover, a different colour can be seen as well on gold electrode. As substrate silicon material was used to support nanowires.

In the result of this paper we can see effectdimension charge on conductancenanowires and electrode that way can see different piezoelectric with silicon substrate due, is silicon material is high piezoelectric and need to

electrodes can accept to current moving normal to elucidate whether can use parameters of piezoelectric model, the flow rate was changed. As shown in Figure 3, at a higher flow rate, faster onset kinetics in the wire response was obtained. The result indicates that the mass transport of mobile analyze is mainly responsible for the obtained wire response. It is also notable that, at a slower flow rate, a significantly 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 higher wires response signal so as to generate a higher signal.

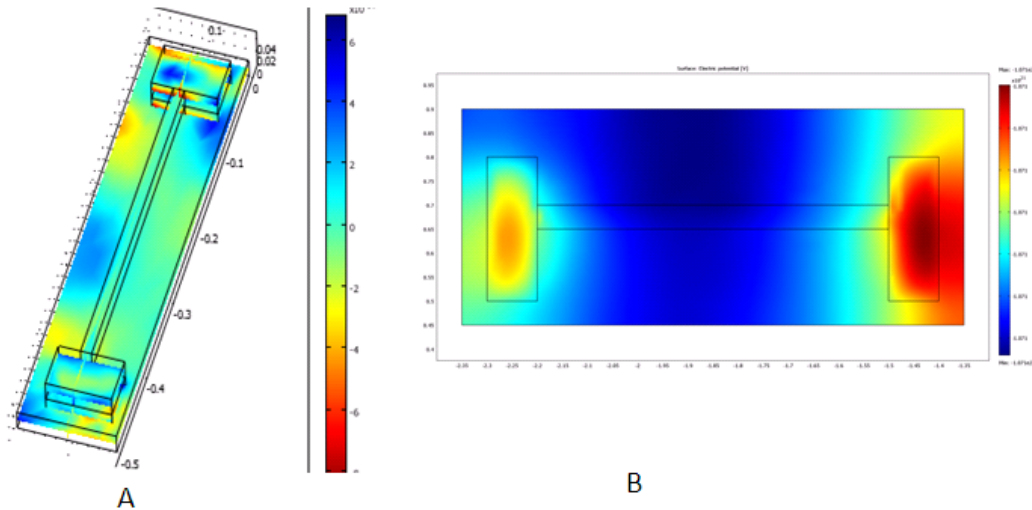


Fig. 2a: Showing Structure 3D dimensions of silicon nanowire with electrode, b) 2D of electrical potential of Silicon nanowire.

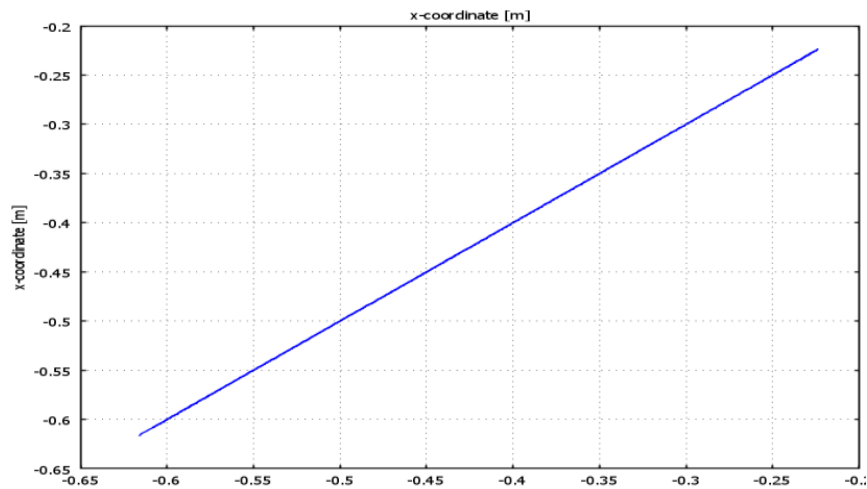


Fig. 3: Showing Analysis Of Dimensions Silicon Nanowire Width.

4. Conclusion:

We simulated a 2D and 3D design and simulation of a silicon nanowire surface using piezoelectric equations to quantitatively validate the existing experimental data for DNA application. The present design is a first step in the nanowires- gold electrode coupling with a detailed electro-chemical model of nanowires. It is observed that the diameter and length of the wire and width affects the charge distribution. A detailed study of these effects upon variations can be performed. The parameters of piezoelectric equations effect the different phases of wire dimension, its initiation and distribution.

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