Contents list available at **IJND**

International Journal of Nano Dimension

Journal homepage: *www.IJND.ir*

A simulation study on the performance of various label-free electronic biosensors

ABSTRACT

K. Talukdar[1],*
A. K. Mitra[2]

[1]Department of Physics, NIT
  Durgapur, West Bengal, India
[2]Department of Physics, NIT
  Durgapur, West Bengal, India.

The efficient detection of charged biomolecules by biosensor with appropriate semiconducting nanomaterials and with optimum device geometry has caught tremendous research interest in the present decade. Here, the performance of various label-free electronic biosensors to detect bio-molecules is investigated by simulation technique. Silicon nanowire sensor, nanosphere sensor and double gate field effect transistor (DGFET) sensor with different device parameters are reported here and their performances are compared. For the three types of sensors, radius of the nanowire, radius of the nanosphere and the silicon body thickness for the DGFET are varied to compare their selectivity, sensitivity, settling time etc. The result of adjustment of the flow of the fluid is also investigated by simulation.

Keywords: *Biosensor; Label-free; Selectivity; Sensitivity; Simulation.*

INTRODUCTION

The nanometer size of the materials provides them large fraction of surface atoms, high surface energy; spatial confinement and reduced imperfections, which do not exist in the corresponding bulk materials. Large surface to volume ratio, large area per mole, increase of the mobility of the electrons near the surface of the material, these are the characteristic features of the nanomaterials. For these reasons, nanomaterials in the form of wires or spheres with their surface functionalized by suitable receptor molecules have caught a great attention for their potential biosensing applications compared to the so-called ELISA technique. But till now, this conventional technique is used for commercial purpose in a large extent in spite of some difficulties of the method such as the long settling time and less sensitivity. The future prospect of the biomedical applications of the nanomaterials depends on the extraordinary electrical, mechanical, thermal and catalytic properties of the nanomaterials along with their biocompatibility and also on their ability to bind with different chemical species [1].

* Corresponding author:
K.Talukdar
Department of Physics, NIT
Durgapur, West Bengal, India
Tel +91 9732107726
Fax +91 3432573894
Email keka.talukdar@yahoo.co.in

Archive of SID

Biomolecules have dimension similar to the nanoparticles. So they can be detected by the nanoparticles in an electrochemical sensor. The review of Vestergaard et al. [2] and Yogeswaran & Chen [3] gives a detailed insight about the electrochemical bio sensors. Nanosphere [4] or nanowires [5] can be used for biosensing purpose. The performance of field-effect transistor (FET) and metal oxide field effect transistor (MOSFET) type biosensors are also reported in some studies [6, 7, 8]. Graphene [9] and carbon nanotubes [10] can also be exploited for biosensing purposes. Again, silver nanoparticles have unique optical, electrical and thermal properties. They can be used in biosensors as biological tags for quantitative detection, in wound dressings, cosmetics, microbial coatings for their antibacterial properties. Biomedical devices containing silver nanoparticles provide protection against bacteria. Their size, shape, surface and aggregation state change while involving a specific target cell and thus provide changed performances. Ag-nanoparticles which have been used for medical interest interact with the cells or microbes by releasing low level of silver ions from their surface. The release rate depends on nanoparticle size, temperature, and exposure to oxygen, sulphur and light. For these advantages silver nanoparticles are used for different biosensing applications [11, 12].

However, modeling and simulation in the field of nanotechnology has been paid attention for its capacity to incorporate diversified system constraints in various fields of application. To develop fundamental understanding of the relation between the structure of matter in the nanoscale to the properties of materials and devices can be understood by modeling and simulation. Once the relationship is clear, better technique can be developed to fabricate nanodevices with better performance. Baronas et al. [13] showed the way of mathematical modeling towards successful fabrication of electrochemical biosensors. Simulation study on silicon nanowire sensors has also been reported in a number of articles [14, 15, 16]. In the present work, the performance of some label-free silicon nanobiosensors with different device geometry is investigated. This type of work may help potential applications in detecting DNA or peptide. They can also be used in finding toxic agents in food materials [17], basically in liquid form. Detection of specific antigens of some

diseases is possible by suitably functionalizing the sensor surface.

DEVICE ARCHITECTURE

These sensors can detect only the biomolecules carrying charges. The surface of the sensor is first functionalized with receptor molecules of known identity. When biomolecules like DNA are introduced into the sensor volume, they will be captured by the receptor molecules depending on their charge and the excess charge after capture will change the electronic conductivity of the sensor. The change will indicate the presence of complementary target molecules in the fluid. Figure 1 shows the geometry of the sensor.
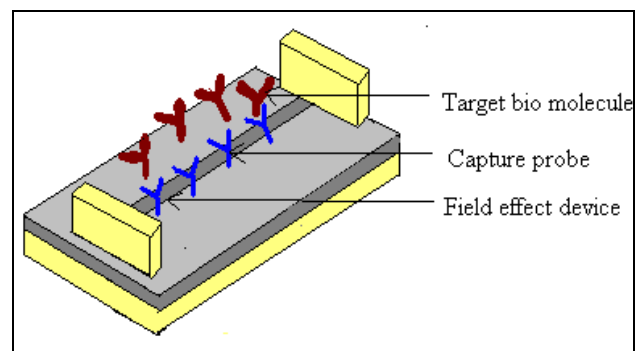

Fig .1. Cylindrical nanowire sensor geometry

The theoretical model is based on self-consistent solutions of Diffusion-Capture model (for the settling time response), Poisson-Boltzmann and Drift-Diffusion Equations (for electrolyte screening and conductance modulation) and the statistical properties of biomolecule adsorption (Selectivity).

RESULTS AND DISCUSSION

Firstly we have varied the radius of the nanowire and found that when the settling time is 3 hour, the minimum analyte density that can be detected is 1.5 x 10-14 M for a wire of radius 50nm. When the radius decreases the sensor becomes more sensitive and the minimum analyte concentration approaches 10-15 (Figure 2). However, the sensor activity does

www.SID.ir

not depend on the length of the wire and a fixed length of 80 nm is used. Here, lower and upper values of analyte concentrations are 1e-15 M and 1e-06 M respectively. The sensitivity of the sensor is depicted in Figures 3, 4 and 5. In these studies we have considered that the test fluid of volume 10 c.c. is injected into the sensor via pipette drop.
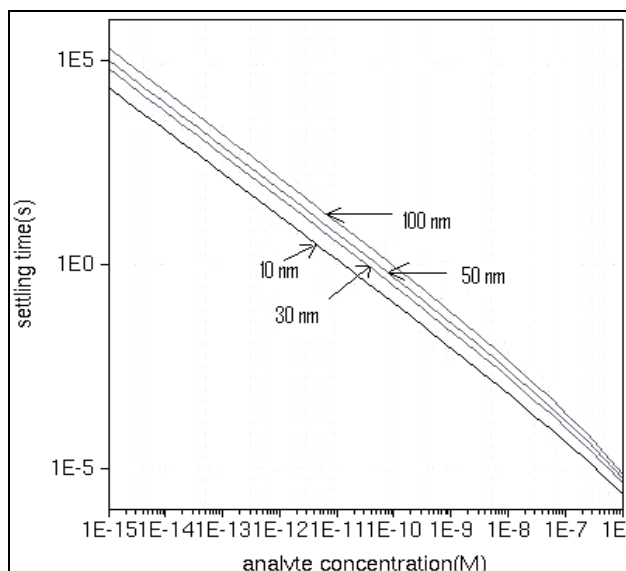

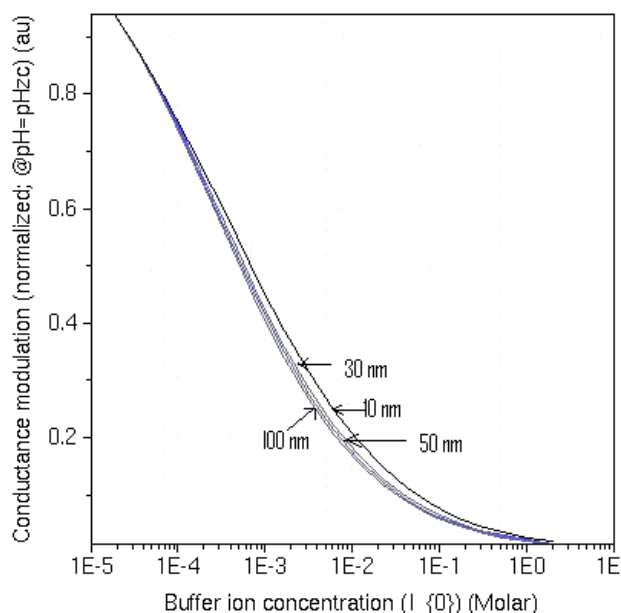**Fig .2.** Settling time vs. analyte concentration of a nanowire sensor

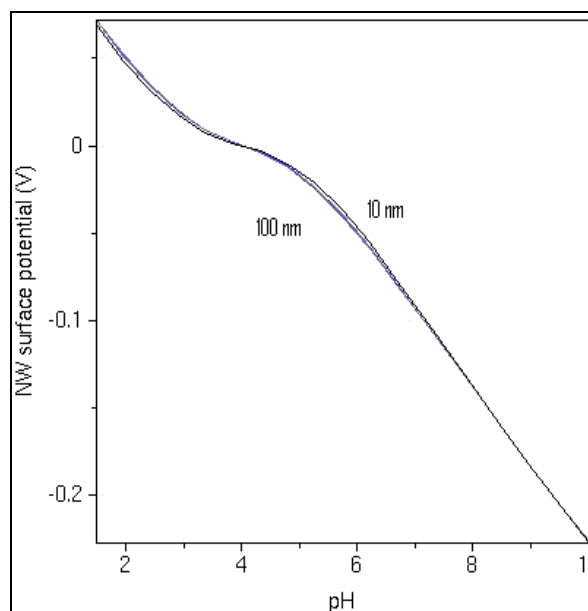**Fig .3.** Conductance modulation vs. buffer ion concentration of a nanowire sensor

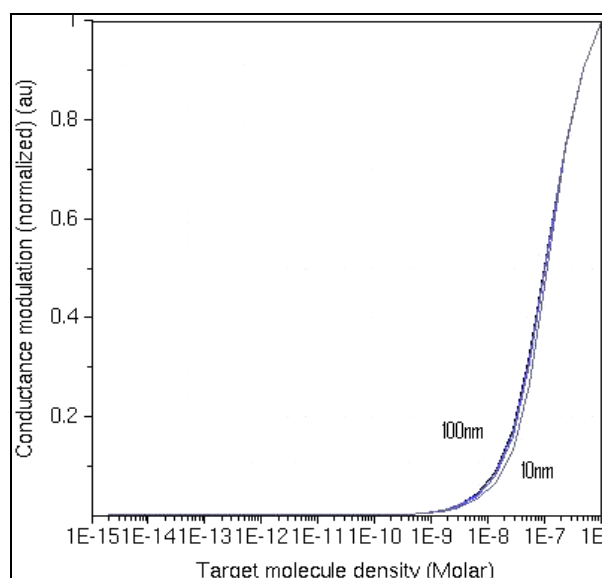**Fig.4.** Conductance modulation vs. pH of a nanowire sensor

Fig.5. Conductance modulation vs. density of the target molecule.

For a given incubation time, sensitivity predicts the surface coverage due to receptor molecules and the Signal-Noise Ratio due to the physisorption of parasitic molecules on the sensor surface (Figure 6). The statistical fluctuations in the arrival time of the analyte molecules on sensor surface can also be estimated and is given in Figure 7.

A nanosphere sensor shows the variation of settling time similar to a nanowire sensor. But it

can detect minimum analyte concentration for a lower incubation period (Figure 8). The lower line is for a nanosphere of diameter 5 nm. For a quantum dot of diameter 5nm, the sufficient decrease of settling time is observed. A minimum analyte concentration of 1.08×10^{-14} M can be detected in only 10.08 second. For the FET type sensor, the silicon body thickness influences the drain current as depicted in Figure 9.
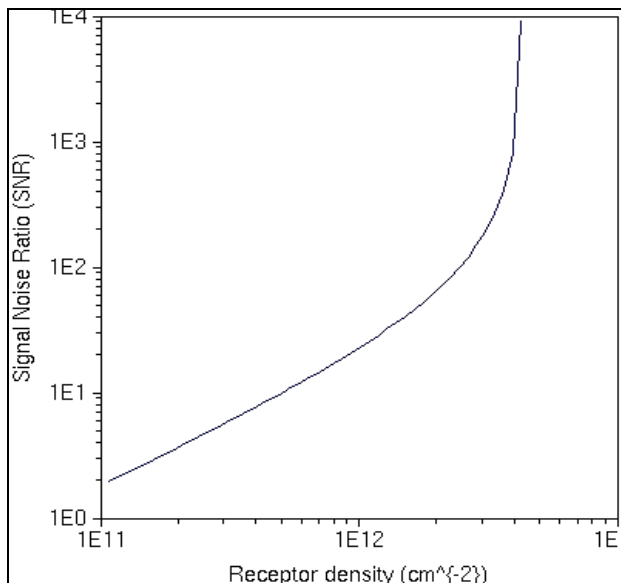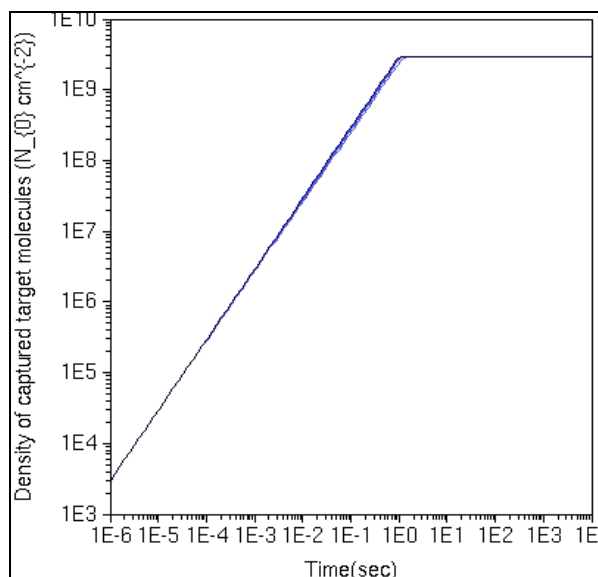

Fig.8. Settling time vs. analyte concentration for a nanosphere sensor

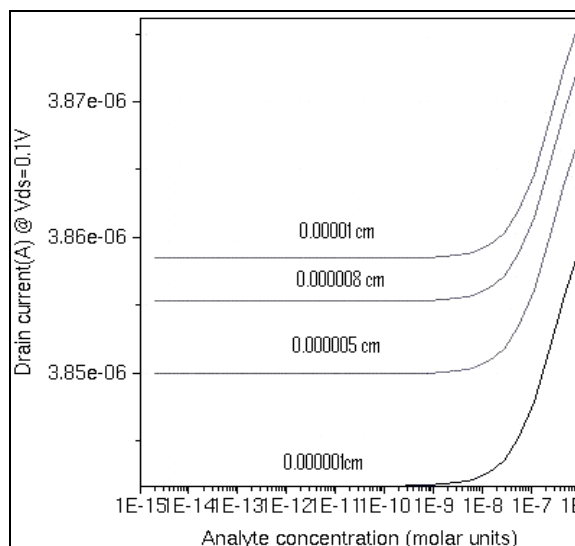**Fig.6.** Signal noise ratio vs. receptor density

Fig.9. Drain current vs. analyte concentration of a DGFET (The value on each curve shows the corresponding value of silicon body thickness)

Fig.7. Density of target molecules vs.incubation time.

By varying the upper and lower values of the analyte concentration, Figure 10 is obtained. The curve is drawn for a nanowire sensor and the sensor is kept in a channel of height and width of 10 cm each and of length 80 cm. The fluid velocity is typically chosen as 50 cm/s. The settling time is changed with the diffusion coefficient of the analyte molecules (Figure 11).
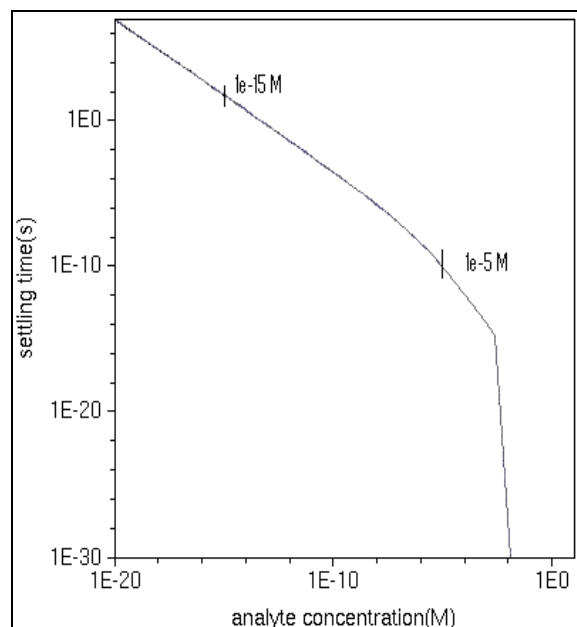
Fig.10. Settling time vs. analyte concentration of a nanowire sensor when fluid is allowed to flow through a channel
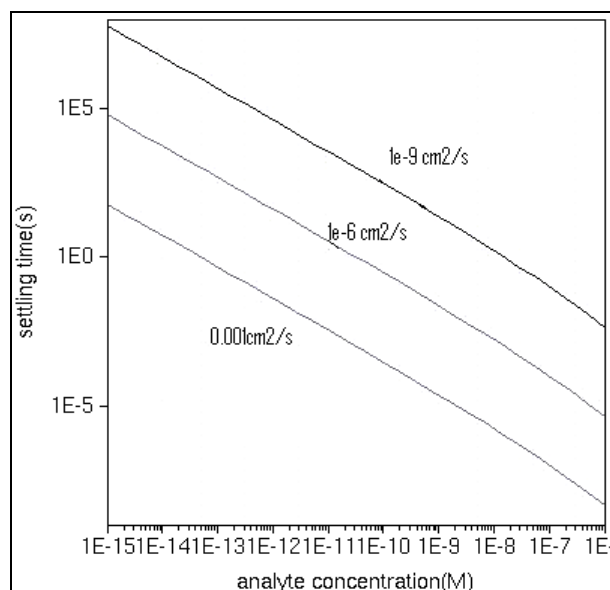

Fig.11. Settling time vs. analyte concentration of a nanowire sensor when fluid is allowed to flow through a channel for different diffusion coefficient of the analyte

CONCLUSION

The performance of various label-free electronic biosensors is studied which can efficiently detect charged biomolecules near the sensor surface by electrostatic interaction. The settling time is found to vary with radius of the nanosphere or the nanowire and the drain current is changed considerably with the radius of the silicon nanowire in the FET. The flow of fluid and the diffusion coefficient of the analyte molecules have also pronounced effect on the performance of the sensors. Sufficient reduction of settling time is reported for a nanosphere of dimension 5nm. So, in vivo detection of charged biomolecules is efficiently done by adjusting the device parameters properly by the above technique.

REFERENCES

[1]   Chiu T.C., & Huang C.C. (2009). Aptamer-Functionalized Nano-Biosensors. *Sensors*, 9, 10356-10388.

[2]   Vestergaard, M.D., Kerman, K., & Tamiya, E. (2007). An Overview of Label-free Electrochemical Protein Sensors. *Sensors*, 7, 3442-3458.

[3]   Yogeswaran U., & Chen S.M. (2008). A review on the electrochemical sensors and biosensors composed of nanowires as sensing material. *Sensors*, 8, 290-313.

[4]   Maxwell, D.J., Taylor, J.R., & Nie, S. (2002). Self-Assembled Nanoparticle Probes for Recognition and Detection of Biomolecules. *JACS*. 124; 9606-9612.

[5]   Wanekaya A.K., Chen W., Myung N.V., & Mulchandani A. (2006). Nanowire- based electrochemical biosensors. *Electroanalysis*, 18, 533-550.

[6]   Ooe, K.; Hamamoto, Y.; Kadokawa, T. & Hirano Y. (2008). Development of the MOSFET type enzyme biosensor using GOx and ChOx. *Journal of Robotics and Mechatronics*, 20; 38-46.

[7]   Kim, D.S., Park, H.J., Park. J.E., Shin, J.K., Kang, S.W., Seo, H.I., & Lim, G. (2005). MOSFET-Type Biosensor for Detection of Streptavidin–Biotin Protein Complexes. *Sensors and Materials*, 17, 259- 268.

[8]   Ahn J.H., Choi S.J., Han J.W., Park, T.J., Lee S.Y., & Choi Y K. (2010). Double- Gate Nanowire field effect Transistor for a biosensor. *Nano Letters*, 10, 2934- 2938.

[9] Shao Y., Wang J., Wu H., Liu J., Aksay I. A., & Lin Y. (2010). Graphene based electrochemical sensors and biosensors: A review. *Electroanalysis*, 22, 1027-1036.

[10] Wang J. (2005). Carbon- nanotube based electrochemical biosensors: A review. *Electroanalysis*, 17,7-14.

[11] Ryu S.W., Kim C.H., Han J.W., Kim, C.J., Jung C., Park H.G., & Choi Y.K. (2010). Gold nanoparticle embedded silicon nanowire biosensor for applications of label- free DNA detection. *Biosensors and Biolelectronics*, 25, 2182-2185.

[12] Zheng G., Gao, X.P.A., & Lieber C.M. Frequency domain detection of biomolecules using silicon nanowire biosensors. *Nano Letters* 10, 3179-3183.

[13] Abad, J. M., Mertens, S. F. L., Pita, M., Fernandez, V. M., Schiffrin, D. J. (2005) "Functionalization of Thioctic Acid-Capped Gold Nanoparticles for Specific Immobilization of Histidine-Tagged Proteins." *J. Am. Chem. Soc*., 127(2): 5689-5694.

[14] Baronas R., Ivanauskas F., & Kulys J. (2010). Mathematical modeling of biosensors an introduction for Chemists and Mathematicians. Springer Dordrecht, Heidelberg, London, New York.

[15] Nair, P., & Alam, M. (2007). Design Considerations of Silicon Nanowire Biosensors. *IEEE T-ED*, 54, 3400-3408.

[16] Nair, P., & Alam, M. (2008). Screenibg-limited response of nanobiosensors. *Nano Letters*, 8, 1281-1285.

[17] Tan, S.J., Lao, I.K., & Ji, H.M. (2006). Microfluidic design for bio-sample delivery to silicon nanowire biosensor - a simulation study. *Journal of Physics Conference Series* 34, 626.

[18] Yalcin B., & Otles S. (2010). Nanobiosensor and food pathogen interaction mechanisms. *Electronic Journal of Environmental, Agricultural and Food Chemistry*. 9, 1257-1273.