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Simulations of silicon nanowire sensor and an integrated smart bio-nano sensor

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Abstract

Background: Simulation-based nano biosensors have been introduced in recent times that will provide a model for the researchers to verify various critical functions of them, which could effectively save time, money, and effort.

Materials and Methods: In this study, we have performed simulations of a silicon nanowire (Si-NW) biosensor, and its various parameters were evaluated. This silicon sensor was designed using the BiosensorLab tool, a simulator from the nanohub website. This paper also presented an Integrated Smart Bio-nano Sensor. The motivation behind this smart sensor was that an incident happened in one of the southern states of India, in the year 2020; the leakage of styrene gas (C_8H_8) from the Polymers industry caused 12 deaths and several people hospitalized. Most people died after they inhaled styrene gas because they thought the pungent smell (of styrene gas) was also part of their kitchen's emissions. This incident prompted us to propose an Integrated Smart Bio-nano Sensor.

Results: The proposed sensor was capable of classifying the origin of sources of emissions dynamically (smart), even under lower concentrations of gas levels (25 ppm) and could alert the habitants in case of untoward danger.

Conclusions: After verifying settling time vs. analyte concentration, the density of captured target molecules concentration with time vs. time, and the signal-to-noise ratio (SNR) of the biosensor in the presence of parasitic molecules vs. receptor density, it was concluded that these three parameters have helped in identifying the characteristics of the proposed bio-nano sensor.

Keywords: Bio-nano Sensors, Volatile Organic Compounds, Integrated Smart Nano sensor, Simulations.

1. Introduction

A biosensor, like any other sensor, is a transducer that converts the biological response to the corresponding electrical signal. Nevertheless, unlike conventional sensors, a biosensor must be highly specific, independent of physical parameters including stirring, temperature, pH, etc. It must also be tiny, bio-degradable, and bio-compatible, which is highly sought after, particularly, in tissue engineering and regenerative medicine [1]. The word biosensor was first coined by Leland C. Clark Jr. [2], an American scientist who is considered the 'Father of Biosensors'. A Clark electrode is a device used to measure oxygen levels in the blood, water, and other liquids.

The combination of nanomaterials and biosensors provides opportunities for building up a new generation of biosensor technologies. Nanomaterials improve mechanical, electro-chemical, optical, and magnetic properties of biosensors and are developing towards single-molecule biosensors with high throughput biosensor arrays. However, because biological molecules have unique structures and properties, it is currently difficult to fully combine these properties with those of nanomaterials and biomolecules to create single-molecule multifunctional nanocomposites, nanofilms, and nanoelectrodes. Other significant challenges for the currently available techniques include processing, characterization, interface issues, the availability of high-quality nanomaterials, tailoring of nanomaterials, and the mechanisms governing the behaviour of these nanoscale composites on the surface of electrodes.

Nano biosensors will play a significant role in combating various grim infections since nanoscience-based materials have different interesting properties than their macro-sized counterparts. Nano-based biosensors would offer excellent avenues as they have unique properties such as enhanced absorption and scattering, relatively profound biocompatibility, facile synthesis [3], and other important characteristics.

In addition, silicon-based biosensors have been recognized as the most relevant sensors to detect DNA, proteins, pH levels, etc. [4]. Various critical features of nano biosensors such as self-powering, re-usability, and long-term stability have been reported in the literature. It has been reported that it has become possible to detect specific sequences of DNA (double-stranded) and RNA (single-stranded) with nanowire biosensors [5]. Kumar and Rao [6] critically evaluated biosensors' physical parameters, including planar biosensors, cylindrical nanowire, nanosphere, extended gate, magnetic particle, pH, and Flexure FET sensors. It was found that the silicon nanowire (Si-NW) average response time is much higher than the ion-sensitive field-effect transistor (ISFET) [7].

Recently, simulation-based nano biosensors were introduced, and they provide a model for the researchers to verify various critical functions. They could effectively save time, money, and effort. This research has, therefore, relied on such simulations to design biosensors. Later, various physical parameters of biosensors were evaluated. This study also proposed an integrated bio-nano sensor.

2. Materials and methods

2.1 Si-NW sensor design

Silicon nanowire sensor was designed using the biosensorLab tool, a simulator from nanoHub.org, developed by the Purdue University (USA) researchers available for research activities at. www.nanoHub.org. Figure 1 depicts a Si-NW sensor. Apart from nanowire (cylindrical) biosensors, there are 'n' of biosensors simulated by researchers from Purdue University, and it is also possible to access various physical parameters of the biosensors. Table 1 shows the different sets of parameters that have been selected for the nanowire sensor simulations.

As far as the nano-based DNA biosensor working principle is concerned, the sensor consists of a field-effect device with a functionalized surface with capture probe (receptor) molecules [8]. If the target molecules diffuse through the solution and reach the so-called field-effect device and get captured by the receptors thereby binding close to the surface. Many biomolecules carry an electrostatic charge under normal physiological conditions. For example, DNA is negatively charged while the net charge of a protein molecule depends on the pH of the solution. The Coulomb interaction between the charge of the target biomolecule and the field device can result in a change in conductivity of the latter and such changes can be measured at the output of the biosensor.

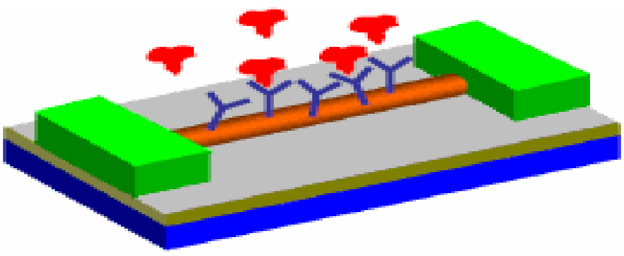

Figure 1. Simulated Si-NW DNA biosensor

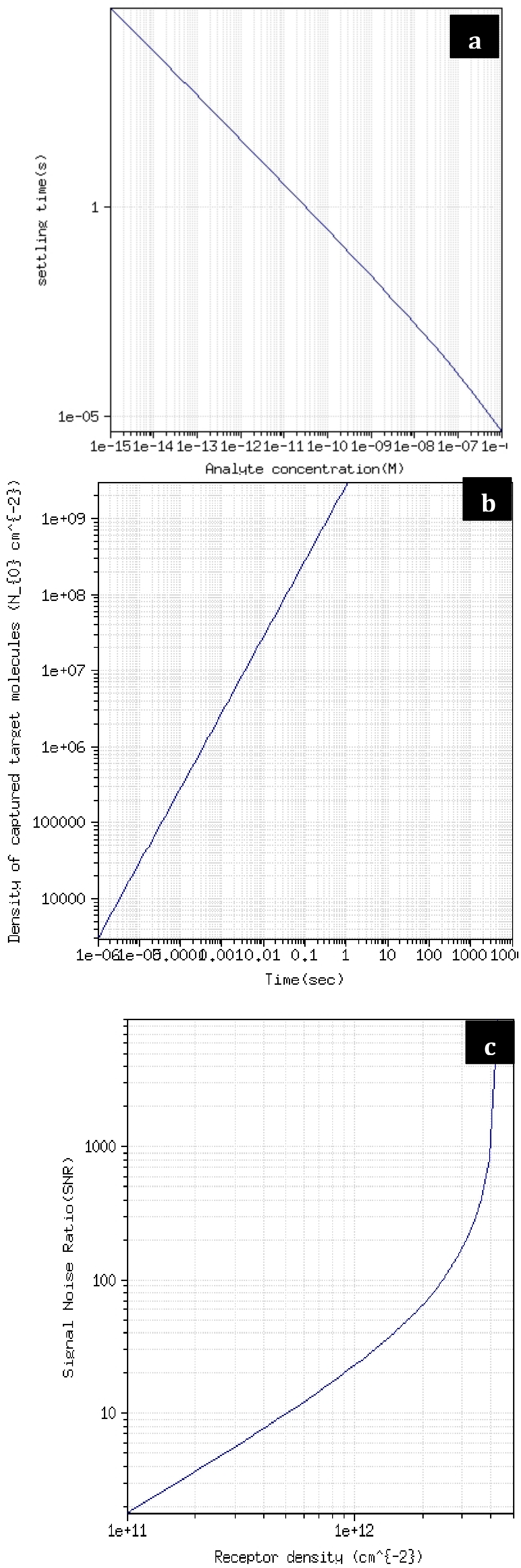

Figure 2. Various physical parameters of the nano biosensor

2.2 Integrated Smart Bio-nano Sensor

Though most of the scientific fraternity is aware of outdoor pollution, which is due to rapid urbanization, indoor pollution would also pose a great threat to the general public. According to the World Health Organization (WHO), the deaths due to both outdoor and indoor pollution are more than double what was documented [9]. Here, we proposed a sensor that can detect three volatile organic components (VOCs including, radon, benzene, and styrene) with higher sensitivity and selectivity, which will, mostly, be used indoors.

3. Results and Discussion

3.1 Si-NW Sensor Design

Based on the experimental model of a nano biosensor, it is required to analyze various properties of the sensor. Figure 2 shows settling time vs analyte concentration (2a), the density of captured target molecules concentration with time vs time (2b), and signal-to-noise ratio (SNR) of the biosensor in the presence of parasitic molecules vs receptor density (2c). These three parameters have helped us in identifying the characteristics of this bio-nano sensor. Further, various iterations (up to 3 steps) of these parameters have been obtained that show the decrease in settling time when concentration increased, and similar trends were also observed in other parameters. The optimum parameters would be, therefore, taken into account in the design of a nanowire-based biosensor.

The simulation of the nanowire sensor has provided a clear view of the pros and cons that would be set as a model for us to overcome various technical glitches while executing a major project. It is also recommended to the scientific community that the scientists at nanoHub have even simulated sensors that might combat recent pandemics i.e., COVID-19, and a serious look at that website may help to create reliable sensors.

3.2 Evaluation of Integrated Smart Bio-nano Sensor

The proposed sensor will consider radon as a template and also choose the radon-related functional device as a monomer, and later Ag-doped $LaFeO_3$ (metal oxide semiconductor perovskite nanomaterial) will be prepared to detect radon gas. Similarly, other gas sensors will be prepared and kept in the same layout, as shown in Figure 3. It can also be observed from the bottom panels of the figures that the response of the sensors in terms of resistivity and concentration. The exciting component concerning this integrated sensor is that it'll have a Field Programmable Gate Array (FPGA), which changes its modus operandi in line with the chaotic state of affairs. The chaotic state of affairs might be an unexpected launch of butane within side the kitchen, risky gas leakage from a chemical factory, and a few unknown stinky chemical emissions.

The large specific surface areas (which increase the interaction between the sensor surface and the surrounding gases), the high porosity, and the useful thickness of the depletion layer are a few advantages of nanomaterials [10]. The proposed sensors work as conventional mere chemiresistive- gas sensors [11]. However, more than a 10-detector array design has already been presented by [12]. But, a sensor that could detect extremely low levels of the emitted gas concentrations has not yet been developed, to the best of the author's knowledge. Nonetheless, an FPGA-type gas sensor (system-on-chip (SoC)) category has already been proposed [13].

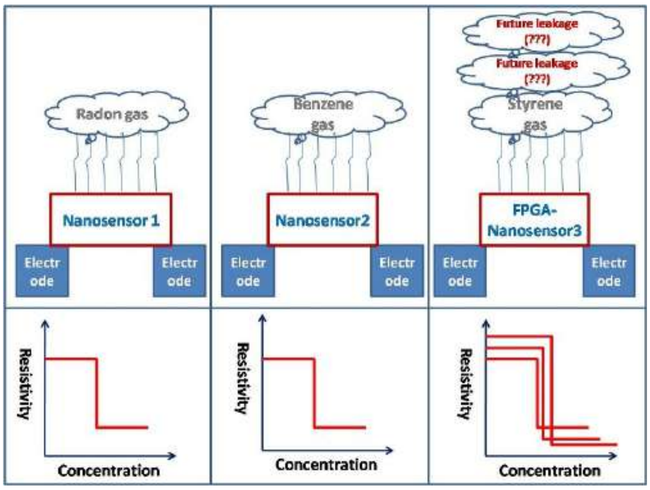

Figure 3. Fabrication schematic of the integrated nano sensor, in which it is also shown an FPGA-based Nano sensor (top right panel), and their responses in terms of resistivity vs concentration.

Figure 4. Dental students working with gas burners in the pre-clinical laboratory.

An unfortunate incident occurred in the early morning hours of 07 May 2020 in one of the southern states of India. There was a leakage of styrene gas from a Polymers firm that led to several deaths and a big number of casualties [14]. Establishing the proposed kind of nano sensors at the industries would be helpful for the early detection of release of any kind of toxic gasses.

These kinds of nano sensors may also be helpful if they are established in dental laboratories, especially in prosthetic labs where large group of students, technicians, and faculty are engaged in making various dental appliances with the usage of gas burners (Figure 4). The leakage of gas may lead to a chaotic situation in the labs. Therefore, this study suggests evaluating the scope of these nano sensors in the dental laboratories.

Future work will be focusing on clarifying the mechanism of interaction between nanomaterials and biomolecules on the surface of electrodes or nanofilms. By using novel properties and emergence of new kind of diseases, it is planned to simulate and later fabricate a new generation of biosensors that could produce results in less time.

4. Conclusion

This study performed simulations of a silicon nanowire biosensor and we also present an Integrated Smart Bio-nano Sensor. The proposed integrated Bio-nano sensor is capable of classifying the origin of sources of emissions dynamically (smart), even under lower concentrations of gas levels (25 parts per million, ppm), and could alert the habitants in case of untoward danger. Various parameters including, settling time vs analyte concentration, the density of captured target molecules concentration with time vs. time and the signal-to-noise ratio (SNR) of the simulated silicon nanowire biosensor have helped in identifying the characteristics of the proposed bio-nano sensor.

Conflicts of interest: Authors declared no conflicts of interest.

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