# Impact of Quantum Mechanical Effects on Silicon Nanowire Biosensors

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## I. Introduction

Due to the superior surface to volume ratio, silicon nanowire (Si-NW) is a good candidate for a direct label-free ultra-sensitive biosensor and [1]-[2]. Compared with the ion-sensitive field effect transistors (ISFÊT), the detection limit of Si-NW biosensors is three to four orders of magnitude higher [3]. Hence, the size of Si-NW biosensors has been progressively reduced to nanometer scale for larger surface to volume ratio and better performance. When the diameter of Si-NW ~10 below biosensors nanometer. the is quantum-mechanical effect may play an important role. In this work, we investigate the impact of quantum effects on the sensitivity performance and device design of Si-NW biosensors.

### **II. Results and Discussion**

Fig. 1 shows the detecting system of a Si-NW biosensor. The detecting system consists of two electrodes (source and drain) and a functionalized surface around the channel. The conductivity  $(G_0)$  of Si-NW biosensors has a change  $\Delta$  G when the functionalized surface with specified receptors conjugates the target biomolecules. The sensitivity of Si-NW biosensors can be defined as:  $S = \Delta G / G_0$ . Fig. 2 is the simulation flow for Si-NW biosensors with and without considering solution bias [6]. Utilizing our simulation flow can easily evaluate the electrical properties of Si-NW biosensors for various design In this work, we consider parameters. the quantum-mechanical effect using the density gradient model [4]-[5]. Fig. 3 shows the calibration between the density gradient model and the exact numerical solution of coupled Poisson-Schrodinger equations.

Fig. 4(a) shows the impact of quantum effects on the sensitivity of Si-NW biosensors with heavy doping. It can be seen that when the diameter scales from 10nm to 3nm, the sensitivity without considering the quantum effect has  $\sim$ 1.37X enhancement. Considering the quantum effect, the enhancement of sensitivity can reach  $\sim$ 1.42X. Fig. 4(b) shows the impact of quantum effects on the sensitivity of Si-NW biosensors with light doping. As the diameter scales from 10nm to 3nm, the sensitivity enhancements with and without considering quantum effects are  $\sim$ 1.13X and  $\sim$ 1.19X, respectively. Even though the sensitivity is boosted more by the quantum effect in the heavily-doped case, it should be noted that the sensitivity for heavily-doped case.

Fig. 5(a) shows a biomolecules-detecting system with electro-diffusion flow [6] which consists of a Si-NW and two biased electrodes. The two biased electrode can generate the electrical field that reduces the number of

mobile ions around the biomolecule. The structure used in our simulation is a 10nm long Si-NW segment as shown in Fig. 5(b). We approximate the DNA on the surface of Si-NW by a small impermeable rod with the backbone charge uniformly distributed and the electron concentration assigned for dsDNA and ssDNA are 2e/nm<sup>3</sup> and 4e/nm<sup>3</sup>, respectively [7]. The distance between the two-side electrodes is 100nm. Other device design parameters are listed in the table of Fig. 5(b). Fig. 6(a) shows that as Si-NW biosensors operate in the accumulation mode without being screening-limited, the induced charge (Q') in the channel increases with solution bias. However, Fig. 6(b) indicates that there exists an optimum solution bias for the largest sensitivity. Fig. 7(a) and Fig. 7(b) show the results for Si-NW biosensors operating in the depletion mode. It can be seen that the Si-NW biosensors operating in the depletion mode exhibit less improvements in sensitivity than operating in the accumulation mode.

Fig. 8 shows that as the diameter scales from 10nm to 7nm, the sensitivity of Si-NW biosensors without considering the quantum effect has a  $\sim 2.5X$  (dsDNA) enhancement, mainly due to the increased surface to volume ratio. When considering the quantum effect, the enhancement in sensitivity can reach  $\sim 3.7X$  (dsDNA). The result indicates that even under the electro-diffusion flow condition, the sensitivity of Si-NWs with smaller diameter can be boosted by quantum effects.

### **III.** Conclusion

We have investigated the impact of quantum-mechanical effects on Si-NW biosensors with small diameter. Our results indicate that by exploiting the quantum effect, the sensitivity of Si-NW biosensors can be enhanced. This study may provide insights for Si-NW biosensors design.

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Fig. 1. Schematic sketch of a Si-NW biosensor.





(a)

+Va/2

(b)

ssDNA and dsDNA are

approximated by a rod

silicor









Fig. 2. Simulation flow for Si-NW biosensors with and without considering solution bias [6].



solution bias (V)

Fig. 6. (a) The induced charge (Q') increases with solution bias. (b) is the corresponding sensitivity. The Si-NW biosensors are operated in the accumulation mode.



Fig. 7. (a) The induced charge (Q') increases with solution bias. (b) is the corresponding sensitivity. The Si-NW biosensors are operated in the depletion mode.

Fig. 8 Impact of quantum mechanical effects on the sensitivity of small diameter Si-NW biosensors.

electro-diffusion

DNA

Design

parameters

channel length

diameter

channel doping

concentration ion

concentration the distance betweer

two side electrode

solution bia:

ds DNA

ss DNA

2.5 3.0

2.0

Fig. 5. (a) Biomolecules-detecting system with

& ssDNA, and the table of device design

electro-diffusion flow[6]. (b) Schematic structure

of a Si-NW with an approximated rod for dsDNA

Si-NW

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