Simulation Approaches of Low-Dimension Structures for Biosensing

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Abstract – **Modeling theory and simulation approaches of field effect transistor (FET)-based sensor for biomolecules detection are presented.**

Keywords – **FET-based biosensor, low-dimension structures, Poisson Equation, Laplace equation.**

I. INTRODUCTION

There are a lot of publications, which describe modeling approaches of low-dimension structures, i.e. simulation of FETs. But modeling of low-dimension structures for biosensing purpose is much more complicated. We have to take into consideration many features. The most difficult is apply biomolecule detection in model.

In this paper, we present a comprehensive modeling theory and simulation approachesto take into account general detection mechanism of molecules bind using FET-based biosensor with low-dimension structures.

II. SIMULATION APPROACHES OF NANOBIOSENSORS

This simulation approach can describe different materials of FET-based biosensorwith the help of following equations: Poisson equation Eq. (1), Laplace equation Eq. (2) and metal equations Eq. (3).

For dielectric description can be used the Poisson Equation as characteristic equation for each point P(x,y,z) in a dielectric, which we write as Eq. (1):

$$\nabla^2 V(x,y,z) = -\frac{r(x,y,z)}{e(x,y,z)} \tag{1}$$

where V(x,y,z) is the electric potential at spatial position P(x,y,z), p(x,y,z) is the electric charge density and ε(x,y,z) is the dielectric constant of the material.

In FET-based biosensor, theelectric charge density is null everywhere except on top of thespacer material on the active area, so Eq. (1) holds on the surfaceof the active area while everywhere else it transforms intoLaplace Equation Eq. (2):

$$\nabla^2 V(x,y,z) = 0 \tag{2}$$

Inside each conductor the electric field isnull, so the potential is constant all over the conductor. Thus,for every point P(x,y,z) of the h-est conductor M_h: V(x,y,z)=Vk

The external electric field is orthogonal to the conductors surface and is given by the following Eq. (3):

$$E_{EXT} = \frac{s}{e}\overset{\mathbf{r}}{n} \tag{3}$$

Forisolated conductors, total charge is set andcannot change, so the integral of surface charge density calculated all over the surface S_{Mh} of conductor M_h has to be constant (Eq. (4)):

$$\int_{S_{Mh}} s\, dS = Q_{Mh} \tag{4}$$

To summarize, we have obtained equations which describe different materials.For this reason, we applied the Finite DifferenceMethod (FDM) to transform the differential equations in linearsystem of equations and problem can be solved applyingnumerical methods [1].

Next approach is based on the numerical solution of Poisson-Boltzmann equation for an electrolyte system.

Using the drift-diffusion charge transport model, the carrier transport in the NWs core can be written as Eq. (5):

$$J_{e.h} = qm_{e.h} n_{e.h} \nabla\Phi \pm qD_{e.h} \nabla n_{e.h} \tag{5}$$

The relationship between the electrostatic potential and the carrier concentrations can be described using Poisson's equation (Eq. (6)) :

$$-\nabla(e_{Si}\nabla\Phi(r)) = q(n_h - n_e + N_D - N_A) \tag{6}$$

In FET-based biosensor, no gate electrode is present and the gate voltage is determined by solving the nonlinear Poisson-Boltzman equation (NPBE) Eq. (7):

$$-\nabla(e_r(r)\nabla\Phi(r)) = r_{fixed}(r) + r_{mobile}(r) \tag{7}$$

In general, the NPBE can only be solved using computational methods due to the rapid exponential nonlinearities, discontinuous coefficients, delta functions, and infinite domain. And the accuracy and stability of the solution to the NPBE is quite sensitive to the boundary layer between the electrolyte and the biomolecules which defines the solvent-accessible surface [2].

III. CONCLUSION

The simulation approach for FET-based biosensor for description of different materials is presented. Another simulation approach based on the numerical solution of Poisson-Boltzmann equation for an electrolyte system is described too.

REFERENCES

[1] M.Barbaro, A.Bonfiglio, "A Charge-Modulated FET for Detection of Biomolecular Processes" *IEEE Trans. on Electron Devices.*, vol. 53, no.1, Jan. 2006, pp.158-165.

[2] Y. Wang, G. Li, "Performance Investigation for a Silicon Nanowire FET Biosensor Using NumericalSimulation", *IEEE Nanotechnology Materials and Devices*, vol. 46, no.2, Oct. 2010, pp.81-86.

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