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Short Communication

Simulation study of the performance of a biologically sensitive field effect transistor

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ABSTRACT

The transformation of biochemical information into a physical or chemical signal is the basic idea behind a biosensor. The efficient detection of charged biomolecules by biosensor with appropriate device has caught tremendous research interest in the present decade. The present work is related to the simulation study of the performance of a functionalized surface of a biologically sensitive field-effect transistor. The detection process is less time consuming and less expensive as it combines a biological sensor and a measurement circuit in a small chip. In this model, a constant potential difference is maintained in between the two electrodes, one of which is functionalized with different types of biomolecules. With the number of double strand DNA oligomers, the concentration of Na^+ and Cl^- ions in the electrolyte in between the electrodes is changed, resulting in changes in surface charge density and dipole moment. Monte-Carlo simulation is performed in a neutral environment after functionalizing one electrode by double strand DNA.

Keywords: *BioFET; Monte-Carlo simulation; Chemical potential; Dipole moment; Ionic concentration; Biosensor.*

INTRODUCTION

In the recent advancement of the biosensors, Field-effect Biosensors (BioFETs) [1-5] are proved to be less costly and easy to design. Theoretical understanding of these field-effect transistors is also necessary to use them in diversified fields like biomedicine, biotechnology, food and drug industry and many others. The reliability of a biosensor must be tested extensively before it is put to practical use. Therefore, proper physical modeling and computer simulations can help to identify the main characteristics, strengths, and weaknesses of a biosensor implementation without the help of any expensive resources, other than computational time. The static and dynamic modeling of a biosensor is explained in detail by Shinwari et al. [6]. The review of Vestergaard et al. [7] and Yogeswaran & Chen [8] gives a detailed insight about the electrochemical bio sensors.

Nanosphere [9] or nanowires [10] 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 [11, 12,13]. Graphene [14] and carbon nanotubes [15] can also be exploited for biosensing purposes. Baronas et al. [16] showed the way of mathematical modeling towards successful fabrication of electrochemical biosensors. A three dimensional modeling of nanowire BioFET is reported by Baumgartner et al. [17]. Finite element modeling is also adopted by Shinwari et al. [18] to simulate a two-dimensional BioFET device. Here we have presented the function of a two-dimensional biofunctionalized surface of a BioFET sensor.

EXPERIMENTAL

Simulation method

The method of simulation is based on Monte-Carlo algorithm in the constant-voltage ensemble developed by Buhlya et al. [19, 20]. The simulations are based on three-dimensional Metropolis Monte-Carlo calculations. The sodium and chlorine ion concentrations are found in the sodium chloride electrolyte between two electrodes, one of which is functionalized with double strand DNA (dsDNA). The whole system is electrically neutral and periodic in the two coordinate directions of the parallel surfaces. The number of nucleotides, the distance between them and the potential difference between the electrodes can be changed which affect the ionic concentration, chemical potential, surface charge density and dipole moment density of the boundary layer at the functionalized surface.

All the parameters of simulation are in nano regime like length of the oligomers, distance between the molecules, linker length etc. Also the biomolecules like dsDNA have dimension in the nano range. The important point is that the height of the simulation cell is also chosen in between 50-100nm. So the scale of our simulation study is nano scale. The scale is shown in Figures 1(a), 2(a) and 3(a) respectively.

Computational model

Ionic interaction with finite atomic size is considered in MC simulation [19]. To create the environment of the real experimental process, several measures are taken. Firstly, in this self-consistent simulation, boundary conditions are used carefully so that the effect of screening effect and large voltages can be included. Secondly, to incorporate low ionic concentration, large simulation domain is set up. Thirdly, mixed size and mixed valance ionic systems are considered for the buffered electrolyte. Lastly, possible rotation of the DNA strands is included. The electrical properties of the biofunctionalized surface of the sensor in the microscopic scale can be solved by this way. Macroscopic behavior of the sensor itself with the microscopic properties can be found i.e. the multiscale problem is handled here by achieving homogenization at the two interface surface. The homogenization problem and a charge transport model help us to find the electric current through the sensor when the charge concentration in the boundary layer has been calculated.

RESULTS AND DISCUSSION

Simulations are performed at a constant voltage. The distance between the molecules, their lengths etc. all are in the nanometer range. The surface charge density and dipole moment of the sensor are found as -0.023755 q/nm^2 and 2.299451 q/nm respectively at a voltage of -50 mV where the DNA strands length is 12 nm. These values change with the number of DNA oligomers and also with the applied voltage. At the same condition, the dipole moment is changed from 0.988380 q/nm to 0.582588 q/nm when voltage is changed from -100 mV to +100 mV respectively. The change of surface charge density is also observed with the change of voltage [Table 1].

When the simulation cell contains 4 dsDNA oligomers and the distance between the molecules is fixed to 6 nm, then at a voltage of -50 mV, the Na^+ and Cl^- ion concentrations vary as depicted in Figure 1(a). Figure 1(b) gives the reduced chemical potential with the iteration step. Here the length of the molecules is 6.08 nm i.e. 12 bases.

Table 1. The change of surface charge density and dipole moment with the change of different simulation parameters

No. of dsDNA oligomers in the cell	Distance between molecules (nm)	Length of molecules (DNA strand length)	Particle No.	Applied Voltage (mV)	Surface charge density (q/nm^2)	Dipole moment (q/nm)
1	8	12	186	-50	-0.023755	2.299451
4	8	12	302	-50	0.080146	1.177237
9	8	12	678	-50	0.068515	1.243713
4	8	16	334	-50	0.137734	1.573042
4	6	12	227	-50	0.173979	1.930458
1	12	12	203	-100	0.010158	0.988380
1	12	12	203	100	-0.104925	0.582588

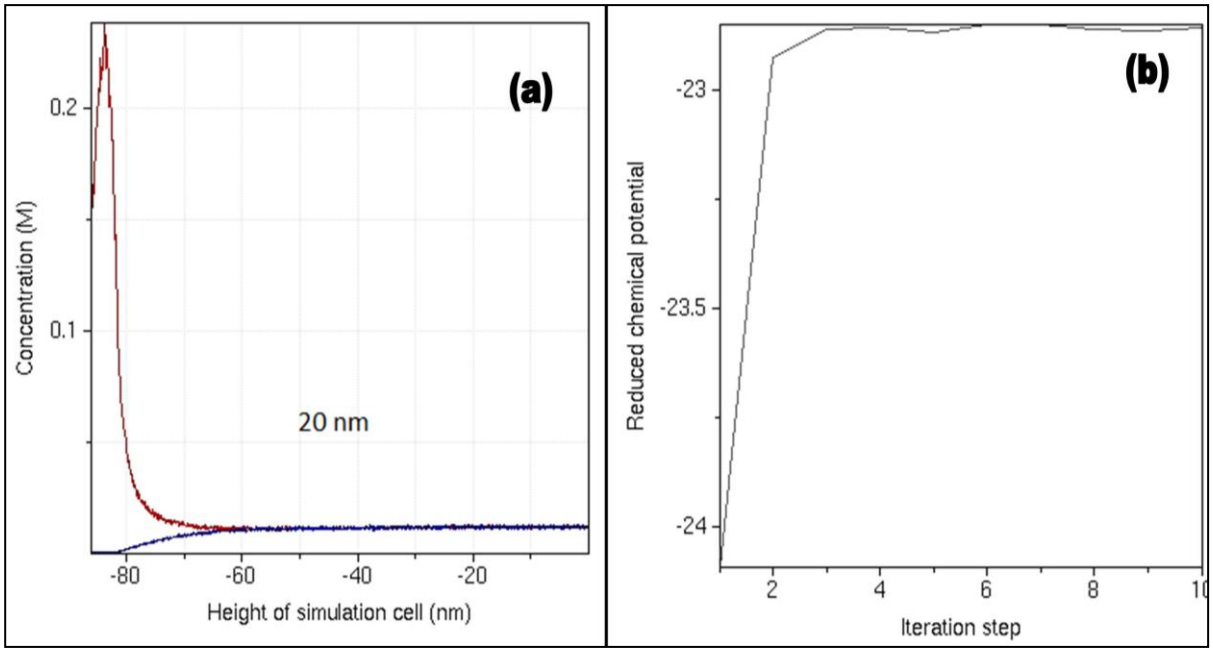

Fig. 1. (a) Na^+ and Cl^- concentration with height of the simulation cell and **(b)** reduced chemical potential with the iteration step when the simulation cell contains 4 dsDNA oligomers with voltage= -50 mV, distance between the molecules=6nm and the length of the molecules is 12 bases.

All the other parameters remaining the same, Figure 2(a) and Figure 2(b) describe the results when the distance between the molecules is 8 nm, and length of the molecules is 7.44 nm i.e. 16 bases.

Again with same conditions of voltage (-50 mV), when the length of the molecules is equal to DNA strand length of 12 nm, the ionic concentration changes as given in Figure 3(a). Here the distance between the molecules is changed to 8 nm. Reduced chemical potential is shown in Figure 3(b) under the same condition.

Table 1 contains the detailed results of simulation.

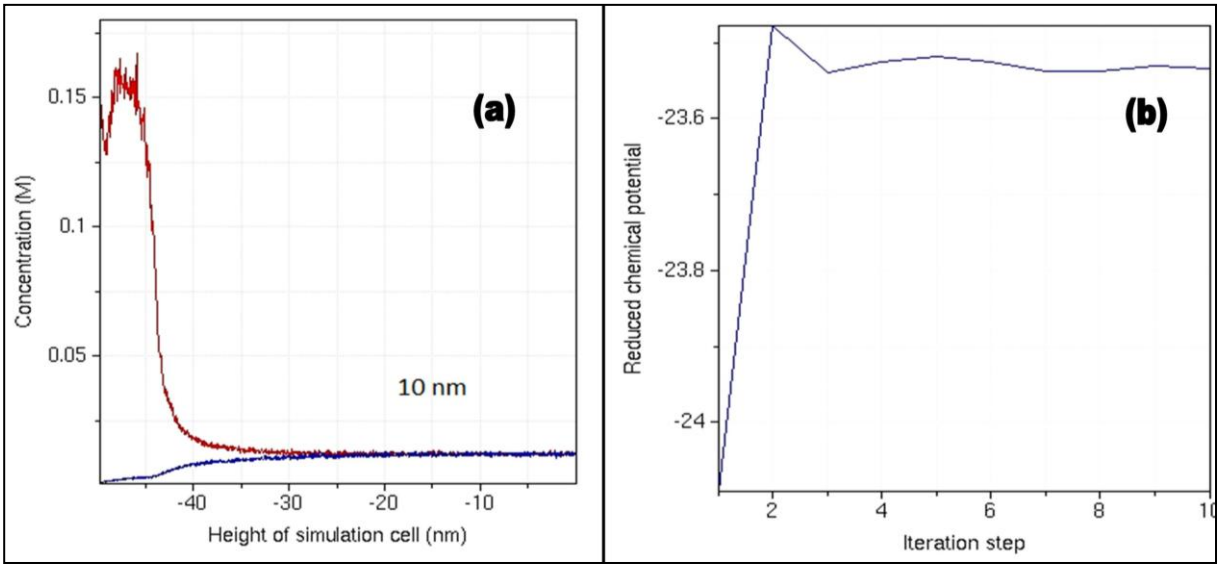

Fig. 2. (a) Na^+ and Cl^- concentration with height of the simulation cell and **(b)** reduced chemical potential with the iteration step when the simulation cell contains 4 dsDNA oligomers with voltage= -50 mV, distance between the molecules=8nm and the length of the molecules is 16 bases.

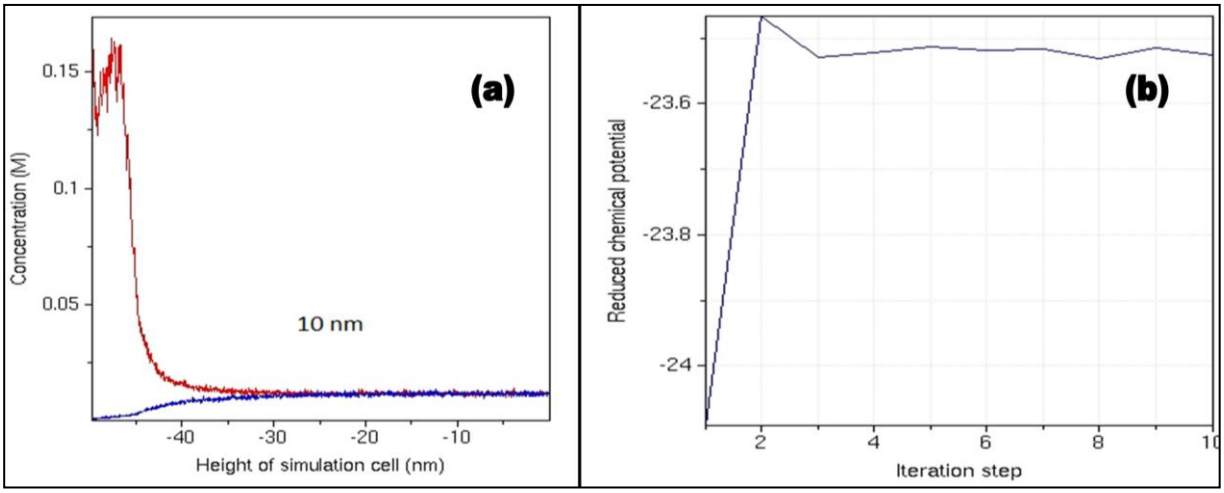

Fig. 3. (a) Na^+ and Cl^- concentration with height of the simulation cell and **(b)** reduced chemical potential with the iteration step when the simulation cell contains 4 dsDNA oligomers with voltage= -50 mV, distance between the molecules=8nm and the length of the molecules is 12 bases.

CONCLUSIONS

The behavior of a bio functionalized surface of a BioFET sensor has been described in the present study. The process can be exploited to investigate systems with low electrolyte concentrations and high surface densities of molecules without involving excessive simulation time. BioFETs are the basis of biochemical sensing devices. But major commercial breakthrough in this field would be possible only after rigorous theoretical studies through simulation technique.

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