Analytic Modeling of BioFET as a pH Sensor

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ABSTRACT

In this paper, the analytic modeling of the BioFET as a pH sensor has been developed from the complete surface potential equation and channel expression. Combining the physical MOSFET theory with electrochemistry of the electrolyte, the expressions of both the potential drop in the electrolyte and the surface potential of the substrate are obtained, respectively, by using an analytic approximation. The drain current and signal noise ratio (SNR) variations with different values of the electrolyte are also discussed for different electrolyte, providing an order condition to gain preferable performance. The modeling results are also verified by the numerical simulation, proving the model validity.

Keywords: device physics, modeling, Bio-FET, pH sensor.

1 INTRODUCTION

Nowadays, the safety of blood and food, et al. is becoming a topical issue which arousing a rapid rising in the study of Biosensor. With the development and improvement of performance of the integrated circuit, BioFET which based on MOSFET is probably cheap and portable in the future. Therefore, BioFET is becoming one of the most promising tools for detecting the biochemical reactions in the electrolyte compared with other biosensors such as polymerase chain-reaction (PVR) and Microarrays [1].

A great deal of work has been done on MOSFET devices to measure chemical quantities since P Bergveld first proposed the concept of BioFET in 1970 [2]. Replacing the conventional gate of the MOSFET with electrolyte and a reference electrode, the device with such a structure is called BioFET which can sense chemical and biological quantities. The simplified diagram of BioFET is shown in Fig.1. Changes in the electrolyte lead to variation of the electrical field, potential and the charge in the semiconductor, thus, this structure is used to monitor ions and concentrations of the solution through the output electrical characteristics of the FET device.

Although the theory of the MOSFET is quite mature, for BioFET study of charge transport in the electrolyte and the electrolyte-semiconductor interface is less reported to our knowledge. This paper focuses on the analytic modeling work on BioFET as a Ph sensor, such as potential drop analysis in the electrolyte and the electrochemistry of the electrolyte-semiconductor interface. The potential drops in the electrolyte and semiconductor are presented in Sec.2 respectively, and the performance characteristics of the BioFET such as the drain current and the signal noise ratio are discussed in Sec.3. Finally, we conclude this paper in Sec.4.
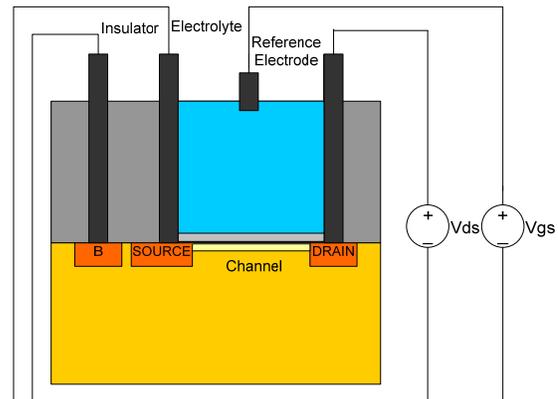
Fig.1 Simplified diagram of the BioFET

2 MODEL DEVELOPMENT

The charge distribution in a solution is shown in Fig.2, and the charge composes of two parts: the surface charge due to site-binding effect Q_{ox} and the diffuse charge in the bulk solution Q_0. A list of the main parameters is presented in TABLE.1. Following the Site-binding model and the Gouy-Chapman-Stern-Graham theory [3], the equations for a 1:1 electrolyte are,

$$Q_{ox} = qNs \frac{\frac{[H_+]_b}{K_a}\exp(-\beta\psi_0) - \frac{K_b}{[H_+]_b}\exp(\beta\psi_0)}{1 + \frac{[H_+]_b}{K_a}\exp(-\beta\psi_0) + \frac{K_b}{[H_+]_b}\exp(\beta\psi_0)} \quad (1)$$

$$Q_0 = -\sqrt{8\varepsilon\varepsilon_{sol}kTc_0}\,\sinh\left(\frac{\beta}{2}\left(\psi_0 + \frac{Q_0}{C_{stern}}\right)\right) \qquad (2)$$

From the basic physical theory of MOSFET, the charge in the silicon substrate is expressed as following,

$$Q_s = \text{sgn}(-\psi_s)\sqrt{2q\varepsilon\varepsilon_{si}N_A}$$
$$\times\sqrt{\beta^{-1}e^{-\beta\psi_s} + \psi_s - \beta^{-1} + e^{-2\beta\phi_F}(\beta^{-1}e^{\beta\psi_s} - \psi_s - \beta^{-1})} \qquad (3)$$

According to the law of electric charge conservation and it is supposed that there is no charge in the insulator, we have

$$Q_{ox} + Q_0 = \Delta Q = -Q_s \qquad (4)$$

ΔQ is much smaller than Q_{ox} and Q_0 in the calculation process, so Eq.(4) is rewritten as

$$Q_{ox} + Q_0 \approx 0 \qquad (5)$$

Symbol	Definition	Value
$[H_+]_b$	Bulk solution concentration	1E-7
β	Thermal voltage	0.026V
Ka	Frist reaction constant	1E-2
Kb	Second reaction constant	1E-7
Ns	Amphoteric site density	5E14 cm^{-2}
C_{stern}	Stern capacitance	20 μF/cm^2
c_0	Solution concentration	1E-3mol/L
ε_{sol}	Electrolyte dielectric constant	78.4
N_t	Volumetric trap density	3E16eV^{-1}cm^{-3}
λ	Tunneling parameter	0.5Å
α	Coulomb scattering coefficient	1.5E5 Vs/C
f	Frequency band	1Hz

TABLE.1 Parmeters for BioFET model
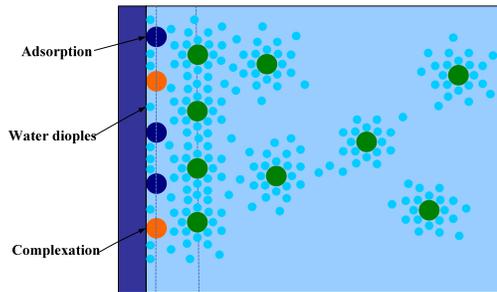
Fig.2. The charge distribution in the electrolyte

Due to the expressions of the charge in solution are rather complicated, the potential drop in the electrolyte is calculated generally in numerical methods. By analyzing the relationship between these various parameters in Eq.(1) and Eq.(2), reasonable approximations are made to obtain a simple analytic expression of the solution surface potential

with acceptable error.

$$Q_{ox} = -qNs\frac{K_b}{[H_+]_b}\exp(\beta\psi_0) \qquad (7)$$

$$Q_0 = \sqrt{2\varepsilon\varepsilon_{sol}kTc_0}\,\exp\left(-\frac{\beta}{2}\left(\psi_0 + \frac{Q_0}{C_{stern}}\right)\right) \qquad (8)$$

The comparison results of Q_{ox} (Eq.(1), (2)) and Q_0 (Eq.(7), Eq.(8)) is shown in Fig.3, which indicates that the approximation adopted in this paper is valid. Substituting Eq.(7) and Eq.(8) into Eq.(5), we have

$$\sqrt{2\varepsilon\varepsilon_{sol}kTc_0}\,\exp\left(-\frac{\beta}{2}\left(\psi_0 + qNs\frac{K_b}{[H_+]_b}\exp(\beta\psi_0)/C_{stern}\right)\right) \qquad (9)$$
$$-qNs\frac{K_b}{[H_+]_b}\exp(\beta\psi_0) = 0$$

Performing the identification transformation of eq.(9) results in

$$3\psi_0 - 2\beta^{-1}\ln A + \frac{qNsK_b}{[H_+]_bC_{stern}}\exp(\beta\psi_0) = 0 \qquad (10)$$

where $A = \dfrac{qNsK_b}{[H_+]_b\sqrt{2q\varepsilon\varepsilon_{sol}kTc_0}}$
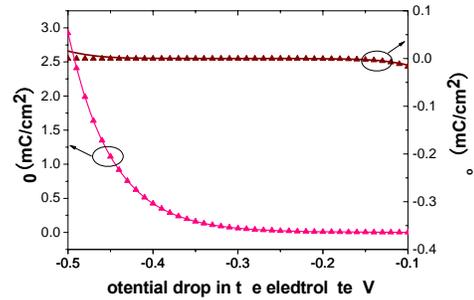
Fig.3 Q_{ox} and Q_0 before(—) and after（＊）approximation

By setting $3B\Psi_0 - 2B\beta^{-1}\ln A = X \qquad (11)$

Eq.(10) is transformed to a familiar formulation and name the result a function, f(X)

$$f(X) = \ln X - \frac{\beta}{3B}X - \frac{2}{3}\ln A = 0 \qquad (12)$$

Where $B = -\dfrac{C_{stern}[H_+]_b}{qNsK_b}$

Eq. (12) appears in many cases and here we choose the analytic approximation to figure it out as mentioned in [4]. Following Fjedly method, an initial value is

$$X_b = \ln[1 + e^{\frac{2}{3}\ln A}]$$

We define,

$$\begin{cases} f = X_b + \ln X_b - \dfrac{2}{3}\ln A \\[2mm] X_0 = X_b\left[1 - f\left(1 - \dfrac{\beta}{3B}X_b + f\left(2(1-\dfrac{\beta}{3B}X_b)\right)^{-1}\right)^{-1}\right] \\[2mm] f_1 = X_0 + \ln X_0 - \dfrac{2}{3}\ln A \end{cases}$$

Finally, the solution is obtained,

$$X = X_0\left[1 - f_1\left(1 - \dfrac{\beta}{3B}X_0 + f_1\left(2(1-\dfrac{\beta}{3B}X_0)\right)^{-1}\right)^{-1}\right] \quad (13)$$

Eq.(11) is rearranged as,

$$\psi_0 = \dfrac{X + 2B\beta^{-1}\ln A}{3B} \quad (14)$$

Substituting (12) into (13), the analytic expression of ψ_0 is obtained. ψ_0 is critical to the sensitivity of the BioFET, and Fig.4 illustrates the potential drop variation in the electrolyte versus the pH values of the solution at different concentrations which shows that the changes of the potential decrease as the solution concentration increases.
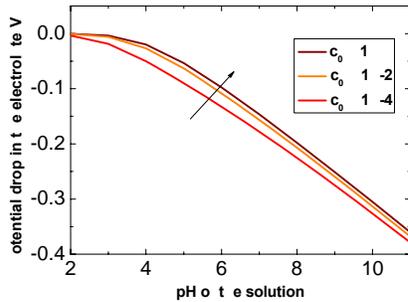
Fig.4 Potential of the electrolyte as a function of the pH value for different solution concentration

Adding the solution potential drop ψ_0 to the potential balance equation of MOSFFT, the expression of ψ_s is given in Eq.(14), where all the symbols have their common physical meanings.

$$V_a - V_{FB} + \psi_0 - \psi_s = \dfrac{\sqrt{2q\varepsilon\varepsilon_{si}N_A}}{C_{ox}}\mathrm{sgn}(\phi) \quad (15)$$

$$\times\sqrt{\begin{aligned}&\beta^{-1}e^{-\beta\psi_s} + \psi_s - \beta^{-1}\\&+e^{2\beta(\phi_F+\phi_n)}(\beta^{-1}e^{\beta\psi_s} - \psi_s - \beta^{-1})\end{aligned}}$$

We define $\begin{cases} C = \mathrm{sgn}(\phi)\dfrac{\sqrt{2q\varepsilon\varepsilon_{si}N_A}}{C_{ox}} \quad A = C\times\sqrt{\beta} \\[2mm] (V_a - V_{FB} + \psi_0)\times\beta = v_a \\[1mm] \beta\psi_s = x_I \\[1mm] \beta\phi_F = x_F \\[1mm] \beta\phi_n = x_n \end{cases}$

Eq.(15) is rewritten in normalized form,

$$v_a - x_I = A\sqrt{e^{-x_I} + x_I - 1 + e^{-2x_f-x_n}(e^{x_I} - x_I - 1)} \quad (16)$$

Eq. (16) shares the same solution with conventional MOSFET, a physical based analytic solution to the MOSFET is used to obtain the surface potential of the semiconductor which modulated by the electrolyte [5]. The normalized surface potential in terms of the W-Lambert function [6] is

$$x_I = \dfrac{x_D + f_I + f_A(1-e^{-x_D})}{1-f_I}$$

$$-W_0\left[\dfrac{f_I}{1-f_I}e^{\frac{x_D + f_I + f_A(1-e^{-x_D})}{1-f_I}}\right] \quad (17)$$

Where, $f_I = f_A e^{-2x_f-x_n}$

$$f_A = A/\left(2\sqrt{v_a\,\mathrm{sgn}(\phi) + A^2/4}\right)$$

$$x_D = \left(v_A\,\mathrm{sgn}(\phi) + \dfrac{A^2}{2}\right) - C\sqrt{v_A\,\mathrm{sgn}(\phi) + A^2/4}$$

The comparison of the proposed analytic solution of the BioFET surface potential with the numerical result of Eq.(15) is shown in Fig.5, which demonstrates that a agreement is achieved. Fig.6 shows the surface potential of the semiconductor at different pH values.
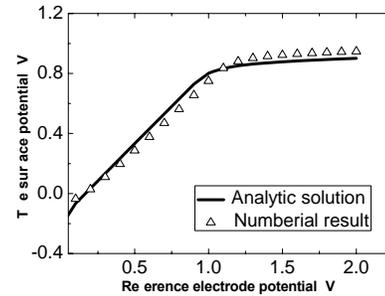
Fig.5 Comparison of the surface potential calculation between the analytic solution and numerical results
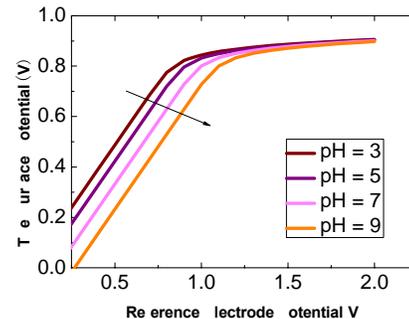
Fig.6 Surface potential of the semiconductor with different pH value

3 RESULTS AND DISCUSSION

It is necessary to discuss the drain current for it is the visual quantity to judge the performance of a device. The surface potential of BioFET is obtained in Sec.2, according to the theory mentioned in [7], the drain current is

$$I_D = \mu \frac{W}{L} \begin{bmatrix} C_{ox}(Va + 2\beta^{-1})(\psi_{SL} - \psi_{S0}) \\ -\frac{1}{2}(\psi_{SL}^2 - \psi_{S0}^2) \end{bmatrix} \quad (18)$$
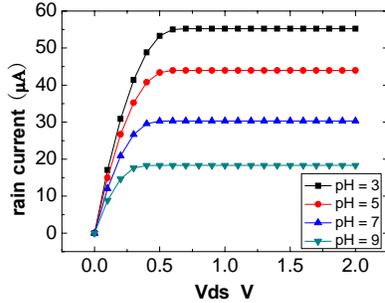
Fig.7 Drain current as a function of the Vds for different pH value

For BioFET, at low frequencies the noise is mainly contributed by both the channel thermal noise and the drain current noise [8].The thermal channel noise is given by

$$S_{V_{Si}} = \frac{4kT\mu_{eff}}{g_m^2 L^2} \left[-C_{ox} \begin{pmatrix} V_a - V_{FB} - \psi_s \\ +\psi_0 + \gamma\sqrt{-\psi_s} \end{pmatrix} \right] \quad (19)$$
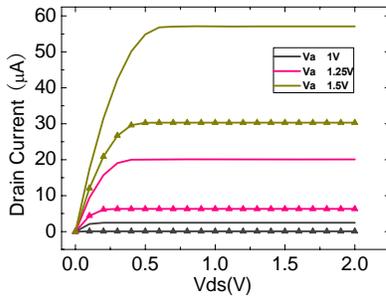
Fig.8 Drain current as a function of the Vds for different reference electrode potential, before (—) and after (▲) the modulation of the electrolyte.

The drain current noise is given by

$$S_{V_g} = \frac{q^2 k T N_t \lambda}{fWLC_{eff}^2} \left[1 + \left(\alpha\mu_{eff} C_{eff} \frac{I_D}{g_m} \right) \right]^2 \quad (20)$$

The currents calculated at different pH values is shown in Fig.7, and Fig.8 demonstrates with a variety of reference electrode potentials before and after the modulation of the electrolyte. The modulation of the electrolyte is significant proves that BioFET has high sensitivity as a pH sensor.
Signal to noise ratio versus the electrode bias potential at different substrate doping level are also given in

Fig.9.Extreme point is in the middle of the curves, which indicates compromise must be made to attain better performance.
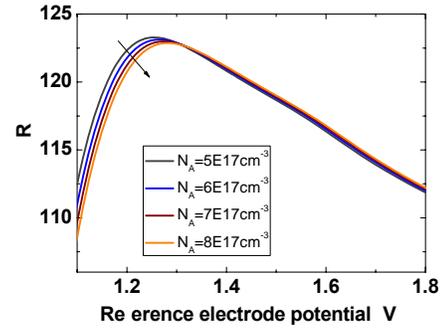
Fig.9 Signal to noise rate at different doping concentration

4 CONCLUSIONS

An analytic model of BioFET is presented in this paper based on expressions of the potential drops in the electrolyte and the surface potential of silicon by using a new analytic approximation. The analytic expressions of the drain current and signal noise ratio (SNR) are also obtained to predict BioFET performance. The devleloped modeling may be useful for us to understand operation of BioFET and the development of the new sensitive sensor.

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