# SURFACE POTENTIAL BEHAVIOR IN ISFET BASED BIO-(CHEMICAL) SENSORS WITH TWO INSULATOR LAYERS IN DARK AND UNDER INTENSITY MODULATED IRRADIATION

### A.V. Surmalyan\* and F.V. Gasparyan

Yerevan State University, Yerevan, Armenia E-mail: amunik@mail.ru

Received 20 October, 2009

# 1. Introduction

Pollution of the natural environment has become one of the major problems in many industrialized countries, which has raised consciousness and understanding of the necessity of environmental care. Consequently, the idea of sustainable development, allowing economical growth and technological progress while protecting the environment, was born. One of the ways of implementing the sustainable growth policy is the creation of specialized networks dedicated for continuous monitoring of the air, water and soil pollution, which employ different kinds of (bio)chemical sensors [1]. The importance of work in this field issued in last years because of increased ISFETs applications. Much works has been recently done to characterize ISFET based on MOS technology [1-4]. Among these devices, proton-sensitive ISFETs are the more deeply analyzed. As is known, the ISFET is in fact nothing else than a MOSFET with the gate connection separated from the chip in the form of a reference electrode inserted in an aqueous solution which is in contact with the gate insulator. ISFET presented in Fig.1 consists of a reference electrode and an insulator layer between which an electrolyte is flowing. The ion concentration in the electrolyte influences the gate potential, which in turn modifies the lateral transistor threshold voltage. In this way, the hydrogen ion concentration exercises an electrostatic control on the drain current mode, which means that the change of the drain current due to the change of the ion concentration in the electrolyte is compensated for by the adjustment of the reference electrode potential [1, 4]. The ISFET sensitivity depends mainly on the choice of the gate material(s). The most commonly used materials are silicon and SiO<sub>2</sub>, Si<sub>3</sub>N<sub>4</sub>, Ta<sub>2</sub>O<sub>5</sub>, and Al<sub>2</sub>O<sub>3</sub>.

Results of analytical investigation of semiconductor surface potential dependency via hydrogen ion concentration, intensity modulated light power (at the LAPS mode operation) and parameters of gate layer(s) in case of complex gate dielectric materials for ISFET based bio-sensor are presented.

# 2. Case of one insulator material

Usually, the ISFET operation is explained by Site-Binding Theory (SBT), which relates the interface potential to pH in the analyzed solution [5]. It is the amphoteric nature of the oxide groups at the interface, in case of SiO<sub>2</sub> these are SiOH groups, which causes the variation of the oxide surface charge at varying pH. The neutral surface hydroxyl site can either bind (SiOH<sub>2</sub><sup>+</sup>) or release (SiO<sup>-</sup>) a proton depending on the solution pH. Because of the binding of the ions with the active sites, the gradient of ion concentration is created in the electrolyte and, according to the Gouy-Chapman-Stern theory the double layer is established at the insulator/electrolyte interface [1, 4]. By utilizing the Gouy-Chapman-Stern theory [6], it can be shown that

$$\varphi_g = \varphi_d + \frac{2kT}{q} \sin^{-1} \left[ \frac{C_h(\varphi_d - \varphi_0)}{\sqrt{\varepsilon_w kTN_{sol}}} \right].$$
(1)

The condition of charge neutrality for the investigated structure (see Fig.1) gives:

$$\sigma_d + \sigma_0 + \sigma_{mos} = 0. \tag{2}$$



Fig.1. ISFET structure.

In Eqns. (1)-(2)  $C_h(\varphi_d - \varphi_0) = \sigma_d$  is the charge density in the diffuse layer,  $C_h$  is Helmholtz layer capacitance per unit area,  $N_{sol}$  is the solution concentration,  $\varepsilon_w$  is the water permittivity,  $\sigma_0$  and  $\sigma_{mos}$  are the charge densities of the surface sites and in the semiconductor given by [3]

$$\sigma_{mos} = \pm \sqrt{2\varepsilon_0 \varepsilon_s kT p_0} \left[ \left( \frac{q \phi_s}{kT} - 1 + \exp\left(-\frac{q \phi_s}{kT}\right) \right) + \frac{n_0}{p_0} \left( -\frac{q \phi_s}{kT} - 1 + \exp\left(\frac{q \phi_s}{kT}\right) \right) \right]^{\frac{1}{2}}, \quad (3)$$

$$\frac{\sigma_0}{qN_s} = \left(\frac{[H_s^+]^2 - K_+K_-}{[H_s^+]^2 + K_+[H_s^+] + K_+K_-}\right)\frac{N_{sil}}{N_s} + \left(\frac{[H_s^+]}{[H_s^+] + K_{N+}}\right)\frac{N_{nit}}{N_s},\tag{4}$$

$$\sigma_d = -\sqrt{8kT\varepsilon_r\varepsilon_0([K_{AK}^+] + [H_s^+])} \sinh\left(\frac{q\varphi_d}{2kT}\right).$$
(5)

Here  $n_0$  and  $p_0$  are the equilibrium concentrations of electrons and holes, respectively,  $N_s$  is the total number of available surface binding sites,  $N_{sil}$  and  $N_{nit}$  are the number of silanol sites and primary amine sites per unit area, respectively,  $K_i$  are the dissociation constants for the chemical reaction at the insulator interface,  $H_s^+$  is the concentration of the protons at the insulator surface,  $\varepsilon_r$  and  $\varepsilon_0$  are electrolyte relative and vacuum dielectric permittivities, correspondingly,  $K_{AK}^+$  is the cation concentration at the common plane.

The solution of the above set of Eqs. (1)–(5) leads to the computation of the dependence of the semiconductor surface potential  $\varphi_s$  on the hydrogen ion concentration (or *pH*):

$$\varphi_{s} = \frac{2kT}{q} \left[ \sqrt{\varepsilon_{s}\varepsilon_{0}kT(n_{0}+p_{0})} \right]^{-1} \left[ \left( \frac{[H_{s}^{+}]^{2}-K_{+}K_{-}}{[H_{s}^{+}]^{2}+K_{+}[H_{s}^{+}]+K_{+}K_{-}} \right) qN_{sil} + \left( \frac{[H_{s}^{+}]}{[H_{s}^{+}]+K_{N+}} \right) qN_{nit} - \frac{q\varphi_{g}}{2kT} \sqrt{2kT\varepsilon_{w}\varepsilon_{0}([K_{AK}^{+}]+[H_{s}^{+}])} + \sqrt{8kT\varepsilon_{0}\sqrt{\varepsilon_{r}\varepsilon_{w}C_{0}\left\{ [K_{AK}^{+}]+[H_{s}^{+}]\right\}}} \right]$$

$$(6)$$



**Fig.2.**  $\varphi_S(pH)$  dependence for different values of the disturbing ion concentrations: pK = -2 and pK = 2.

Semiconductor surface potential *pH*-dependences one the disturbing ion concentrations are presented in Fig. 2. As seen, the disturbing ions cause the characteristics to flatten out for same values of the hydrogen ion concentration. This may be explained taking into account the fact that other ions present in the measured solution, the so-called disturbing ions influence on  $\varphi_s(pH)$ characteristics *pH* sensitivity. The *pH*-sensitivity of ISFETs operating in LAPS mode is determined principally by the *pH*-sensitivity of the layers SiO<sub>2</sub>, Si<sub>3</sub>N<sub>4</sub>, Al<sub>2</sub>O<sub>3</sub>, Ta<sub>2</sub>O<sub>5</sub>. It is shown that at the operation in LAPS mode the semiconductor surface potential can be presented as (6) by multiplying by irradiation factor *L* [7]

$$L = \left(1 + \frac{2\tau W(1-R)\alpha}{h\nu N_a \sqrt{1 + (\omega\tau)^2}}\right)^{-1}$$

where W is the incident irradiation power density, R is the reflection coefficient at the irradiation entrance interface,  $\alpha$  is the irradiation absorption coefficient,  $N_a$  is the concentration of acceptors in p-Si,  $\omega$  is the light modulation frequency,  $\tau$  is the electrons life time.  $\varphi_s(pH)$  dependences for different values of W are presented in Fig.3. As one can see, the semiconductor surface potential is decreasing depending on irradiation power density, what is ordinary. It depends on the variation of carriers concentration caused by generated electron-hole pairs in depletion layer.



**Fig.3.**  $\phi_s(pH)$  dependences at the various irradiation powers for the case pK = 2.

#### 3. Case of two insulator materials

Additionally we have obtained an equation for the case of two different insulator materials

$$\varphi_{s} = -\frac{C}{C_{h}} \left( E_{1}d_{1} + E_{2}d_{2} \right) + \varphi_{d} + \frac{qN_{sil}}{C_{h}} \left( \frac{[H_{s}^{+}]^{2} - K_{+}K_{-}}{[H_{s}^{+}]^{2} + K_{+}[H_{s}^{+}] + K_{+}K_{-}} \right) + \frac{qN_{nit}}{C_{h}} \left( \frac{[H_{s}^{+}]}{[H_{s}^{+}] + K_{N+}} \right), \quad (7)$$

where  $C_h$  is the Helmholtz layer capacitance per unit area, C is the two insulators double layer capacitance  $C = (\varepsilon_0 S/4\pi)\varepsilon_1\varepsilon_2/(\varepsilon_1 d_2 + \varepsilon_2 d_1)$ , S is the insulators surface area,  $\varepsilon_{1,2}$  and  $d_{1,2}$  are the dielectric permittivity and thicknesses of insulators, respectively.

$$\varphi_d = \varphi_g - 2kT/q \sqrt[4]{\varepsilon_w N_{sol} / \varepsilon_r ([H_s^+] + K_{AK}^+)} .$$
(8)

The solution for this case is presented in Fig.4. As seen, in the presence of second dielectric the range of pH-sensitivity changes and increases. For the same value of the surface potential the hydrogen ion concentration was decreased. By changing the gate thickness or insulator types we can obtain the surface potential characteristics capable of pH.

In case of two dielectrics in the presence of intensity modulated irradiation Eq.(8) was multiplied by the factor L. The simulation results for this case are represented in Fig.5. As one can see in Fig.5, the curves are clearly similar. This means that for both cases the dependences of insulator surface potential *pH* are the same, so two dielectrics demonstrate the same characteristics.



Fig.4. pH-dependencies of semiconductor surface potential in case of one and two insulators.



**Fig.5.**  $\phi_s(pH)$  dependencies in case of two insulator pairs (SiO<sub>2</sub>/Ta<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub>/TiO<sub>2</sub>) in presence of intensity modulated irradiation

In Fig.6 are presented surface potential pH-dependences on the disturbing ion concentrations in case of two insulators SiO<sub>2</sub>/TiO<sub>2</sub> in the presence of intensity modulated irradiation for two different irradiation power densities. As we have seen above in Fig.3, the semiconductor surface potential is decreasing depending on irradiation power density in case of one insulator dielectric material. It is clear that, depending on irradiation power, the surface potential characteristics in case of two insulator dielectrics is also changed nearly at the same portion.

In Fig.7 are presented potential dependences for  $SiO_2/TiO_2$  case in the presence and absence of intensity modulated irradiation. The range of sensitivity changes in potential point of view. At the same time the pH-sensitivity range is not changes so much.

Dependences in case of two insulators SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> in the presence and absence of the intensity modulated irradiation are presented in Fig.8. In this case also different characteristics of surface potential behavior and a little change of sensitivity are present.



**Fig.6.**  $\phi_S(pH)$  dependences in case of two insulators SiO<sub>2</sub>/TiO<sub>2</sub> in presence of intensity modulated irradiation: 1 - W = 0.1W, 2 - 0.5W.



**Fig.7.**  $\varphi_S(pH)$  dependencies in case of two insulators SiO<sub>2</sub>/TiO<sub>2</sub> in presence (1) and absence (2) of intensity modulated irradiation.



**Fig.8.**  $\varphi_s(pH)$  dependences in case of two insulators SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> in presence (1) and absence (2) of intensity modulated irradiation.

Dependences in Figs.2–8 are plotted using following parameters for Si, insulators and electrolyte at  $\varphi_g = -0.7$  V and 300K [2, 7, 8]:  $\varepsilon_s = 11.7$ ,  $\varepsilon_w = 78.3$ ,  $\varepsilon_r = 5$ , R = 0,  $\tau = 10^{-6}$  s, ,  $\rho_{Si} = 1\Omega \cdot \text{cm}$  ( $p_0 = N_A = 1.3 \times 10^{16}$  cm<sup>-3</sup>,  $n_0 = 1.73 \times 10^4$  cm<sup>-3</sup>),  $\alpha = 500$  cm<sup>-1</sup>, hv = 1.12 eV,  $N_{Sil} = N_{Nit} = 10^{12}$  cm<sup>-2</sup>,  $N_a = 2.6 \times 10^{15}$  cm<sup>-3</sup>,  $C_H = 4.89 \times 10^{-6}$  F,  $K_+ = 10^2$ ,  $K_- = 10^{-6}$ ,  $K_{N+} = 0.0001$ ,  $K_{AK}^{++} = 0.01$ .

### References

- 1. M. Daniel, M. Janicki, W. Wroblewski, A. Dybko, Z. Brzozka, A. Napieralski. Technical University of Al. Politechniki, 11, 93 (2004).
- 2. M. Janicki, M. Daniel, M. Szermer, A. Napieralski. Microelectronics and Computer Science, Technical University of Al. Politechniki, 11, 93-590 (2004).
- 3. G. Massobrio, S. Martinoia, M. Grattarola. Simulation of semiconductor devices and processes, vol. 4, (1991).
- 4. P. Bergveld. Sensors and Actuators B, 88, 2003.
- 5. D.E. Yates, S. Levine, T.W. Healy. J. Chem. Soc. Faraday Trans., 170, 1807 (1974).
- 6. P.R. Barabash, R.S.C. Cobbold, W.B. Wlodarsdi. IEEE Trans. ED, 34, 1271 (1987).
- 7. F.V. Gasparyan. Sensors and Transducers (in press).
- 8. D. Landheer, G. Aers, W.R. McKinnon, M.J. Deen, et al. J. Appl. Phys., 98, 044701 (2005).