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Modeling of Ion Sensitive Field Effect Transistor for Sensing Application using TCAD

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Abstract: Hydrogen ion concentration (pH) of a solution can be measured using FET type sensor called Ion sensitive field effect transistor, ISFET. Chemical reactions occur at the electrolyte – insulator interface making the FET sensitive to pH. The objective of this work is to model the electrolyte-insulator structure of a transistor using Silvaco TCAD tool. Sensitivity is measured based on the shift in the threshold voltage which is caused by the effect of pH on the charge and the potential distributions in the gate insulator. Based on the analytical calculation of parameters of the electrolyte region, semiconductor materials are used to model the reference electrode and electrolyte. In this study, Silicon Nitride and Aluminum Oxide are used as gate insulators for ISFET and their performance comparison is made for sensing applications. The transfer and output characteristics of the transistor are obtained by simulation for both the films for various thicknesses. A comparison of the effect of thickness of films on device performance is analyzed since the dielectric constant of Aluminum oxide is higher than Silicon nitride.

Keywords: ISFET, Electrolyte-insulator interface, Silvaco, TCAD, Electrolyte model

1. Introduction

Measurement of power of hydrogen(pH) holds great importance for biomedical, environmental and chemical/biochemical applications since most of the chemical reactions are taking place due to change in pH. The traditional device to measure pH is a glass membrane electrode. However, glass membrane electrode comes with some limitations though having better sensitivity such as being fragile, the inability to operate at high temperatures, large size, difficulties in manufacturing, and small life span. However, the concept of Ion Sensitive Field Effect Transistor (ISFET) developed by P. Bergveld in 1970 introduced a remedy for these shortcomings. ISFET provides faster response and is easy to maintain due to the self-cleaning nature of the metal oxide layer. ISFET also provides many more advantages in biomedical applications since arrays of devices for multiple biomarker detection can be developed. Thus, hand-held screening instruments for multiple target detection can be developed cost effectively. ISFETs are compatible with CMOS, work at low power, easy to integrate with read out circuits with added advantage of low input impedance solid state device [1]. Silvaco T-CAD supports process design along with device design. Silicon Nitride and Aluminium Oxide are higher dielectric constant materials compared to Silicon dioxide, which enable thinner layers for the dielectric.

An ion-sensitive field-effect transistor (ISFET) is modelled by removing the gate contact of a MOSFET and replacing it with an electrolyte and reference electrode [2]. Due to the interaction between the ions and the gate oxide, there will be variations in the gate voltage. By measuring the change in gate voltage, the concentration of specific ions in the electrolyte can be determined. The current through the transistor changes when the concentration of ions changes. The need for reference electrode is that to charge the electrolyte insulator structure needs two connections – one in electrolyte and the other in silicon. The electrolyte terminal can be connected to voltage source with the help of reference electrode and now, the metal gate of MOSFET is substituted by both reference electrode and the electrolyte. The gate to source voltage can be taken as the voltage in the reference electrode.

Source and drain are constructed as for the MOSFET. Metal gate electrode is removed so that the underlying insulator layer gets exposed to solution. When there is a change in the concentration of ion in the solution, the threshold voltage gets modulated, and the drain current starts to vary because of the linear relation with threshold voltage. Hence, ISFETs are biased in non-saturated mode during normal operation. Due to its pH sensing capability, it is used in biomedical applications [3]. But achieving high sensitivity is always a challenge. Modelling the relation between sensitivity and sensing film properties could result in improved sensitivity.

Modelling of ISFET is useful in making devices with enhanced sensitivity because this provides the prediction of function of the device for different new sensing materials. After the introduction of the basic model called site-binding model, many researchers have developed many models. The interfacial potential can be given as a function of pH of the solution. In this paper, a model is developed based on the relationship of the form $\Psi 0 = f$ (pH) and check the validity of the model by simulation using TCAD software.

Modelling of processes using Silvaco provides a way to interactively explore the fabrication process, study the effects of process choices and make users to participate in the activity of a "Virtual Wafer Fabrication" factory. The simulation of ISFET structure with silicon nitride and aluminium oxide as sensing films using Silvaco Athena is shown in this paper. The TCAD version used doesn't support modelling of the electrolyte-insulator interface. So, an electrolyte model was developed to mimic the behaviour of reference electrode and the electrolyte-insulator interface [4]. In this work, mapping of the behaviour of cations and anions in the electrolyte region as described by Poisson-Boltzmann equation is done with holes and electrons governed by Fermi-Dirac distribution.

Using Silvaco ATLAS, the transistor is simulated for obtaining output and transfer characteristics [5]. For the simulation, Newton method and Schockley Read Hall (srh) model were used. The thickness of the sensing film was varied and analysed the performance of the transistor.

In literature, sensitivity analysis is done for transistor with silicon nitride sensing film. In this work, a comparison study of transistor with silicon nitride and aluminium oxide sensing films is given and shown that silicon nitride has the best sensitivity.

2. Model for Simulation and Experimental Considerations

The drain current of an ISFET must be chosen to be as that of a normal MOSFET while in a non- saturated region and is given by equation (1).

$$I_D = \frac{\mu_n C_{ox} W}{L}\left[(V_{GS} - V_T)V_{DS} - \frac{1}{2}V_{DS}^2\right] \quad (1)$$

Here, C_{ox} is the capacitance per unit area of the gate is the mobility of electrons in the inverted channel (n-channel transistor), W & L is the channel width and length of ISFET.

The channel inversion in ISFET occurs due to the interface charges between the sensing film and electrolyte as well as the potential applied using reference electrode. Hence, the flat band voltage given by equation (2) includes the effect of the reference electrodes indicated by the term E_{ref} which is the reference electrode potential with respect to the vacuum.

$$V_{FB} = E_{ref} - \Psi_0 + \chi^{sol} - \frac{\phi_{Si}}{q} - \frac{Q_{ss}+Q_{ox}}{C_{ox}} \quad (2)$$

Here Ψ_0 represents surface potential i.e. the potential drop across the bulk of the solution and sensing film, χ^{sol} is a constant which represents the surface dipole potential of the electrolytic solution. Thus, the threshold voltage of ISFET can be expressed as equation (3)

$$V_T = E_{ref} - \Psi_0 + \chi^{sol} - \frac{\phi_{Si}}{q} - \frac{Q_{ss}+Q_{ox}+Q_B}{C_{ox}} + 2\phi_F \quad (3)$$

In equation (3), except Ψ_0, all the terms are constant. The surface potential variation makes the ISFET sensitive to the pH of electrolyte. There is similarity between the equation for cations and anions in the electrolyte solution and equations for holes and electrons in the semiconductor material [6]. Using this relation, an electrolyte model was developed as given in equation (4) and an electrolyte having dielectric constant equivalent to water and band gap=1.5eV [7] can be modeled as a semiconductor with a density of states given by equation (4)

$$N_C = N_V = \begin{cases} 10^{-2} * N_{av}(C_0 + C_{HB}) & pH \leq 7 \\ 10^{-3} * N_{av}\left(C_0 + \frac{10^{-14}}{cH_5}\right) & pH > 7 \end{cases} \quad (4)$$

Here, N_C and N_V are given in cm^{-3}, N_{av} is the Avogadro's number, C_0 (mol/lit) indicates molar concentration of the salt ions in the solution, and C_{HB} is the concentration of hydrogen ion solution when normalized to 1M. The total concentrations of negative and positive charges are represented by n and p respectively.

$$n \cong N_C \, e^{\frac{E_C - E_f}{kT}} \qquad (5)$$

$$p \cong N_V \, e^{\frac{E_f - E_V}{kT}} \qquad (6)$$

The concentration of hydrogen ion solution and molar concentration of salt ions are known, for a given value of pH. By applying these values and Avogadro number in equation (4), N_C and N_V are known. With these values, the concentrations of positive and negative charges are obtained from the equations (5) and (6). Thus, the cations and anions are mapped to electrons and holes. By giving these values to the germanium semiconductor, the electrolyte can be exactly modeled. These values will vary for different values of pH. For each value of pH, the equations are solved, and the values of p and n are calculated.

The structure of ISFET along with the electrodes is shown in figure 1. The n-type germanium semiconductor is used as reference electrode for the purpose of simulation and fabrication in Athena [8]. Gold is used as the contact which replaces the electrolyte solution.

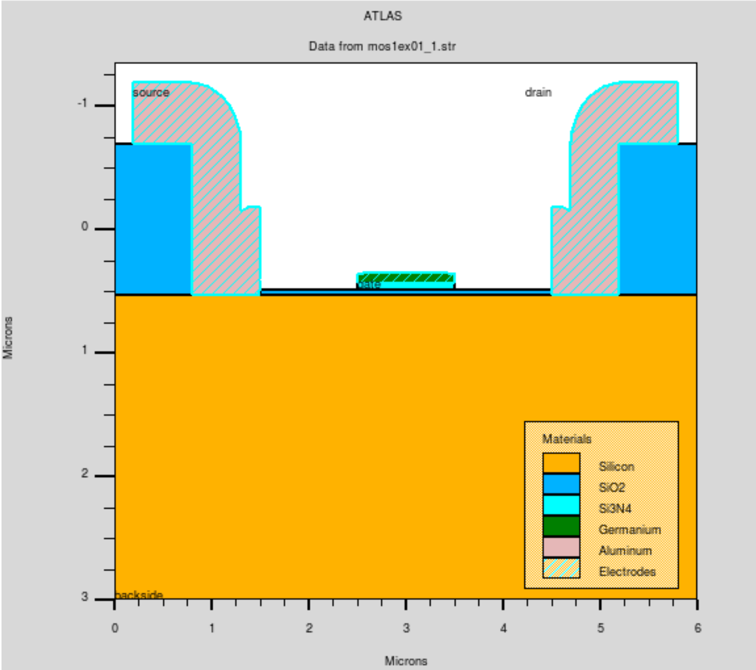

Figure 1. Structure of ISFET with Silicon Nitride sensing film built using Athena.

The doping profile of the transistor is shown in fig 2. The source and drain are constructed by doping phosphorous into the silicon substrate. Here, the thickness of SiO_2 is 50 nm and Si_3N_4 is 80 nm [9].

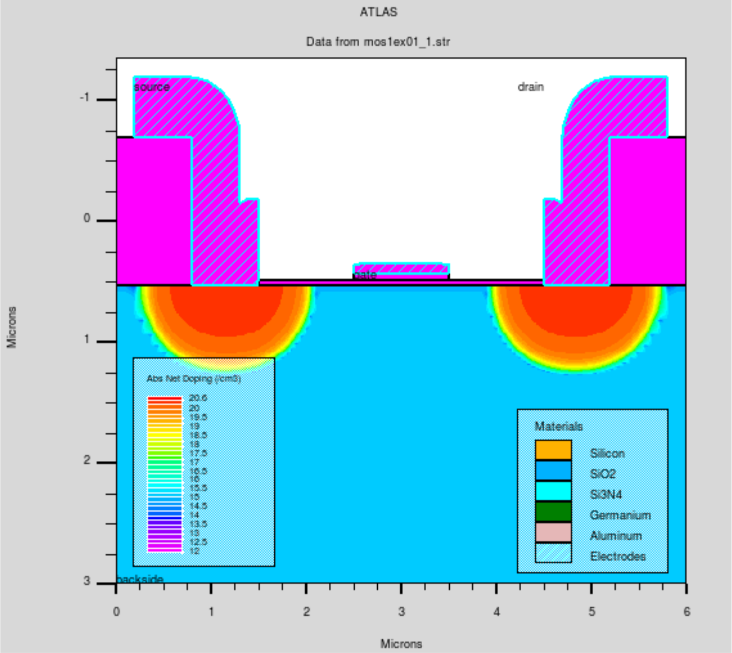

Figure 2. Doping Profile of ISFET with Silicon Nitride sensing film simulated using Athena.

3. Model Simulation and Electrical Characteristics

The transistor constructed in ATHENA is simulated using ATLAS. The transfer and output characteristics of the transistor with 50nm thick silicon nitride film are given in figure 3 and 4. When the gate is biased from 0V to 3V keeping the drain voltage fixed at 0.5V, the drain current increases. The threshold voltage is found to be 0.833V.

When the drain voltage varies from 0V to 3V keeping the gate to source voltage fixed, the drain current increases. The simulation is done for various sensing film thicknesses: 50 nm, 100 nm, 150 nm and 200 nm for pH = 3. It was observed that the threshold voltage increased when the thickness of the film increased. The same transistor is simulated with Silicon oxide as sensing film and outputs are obtained for 4 different thicknesses.

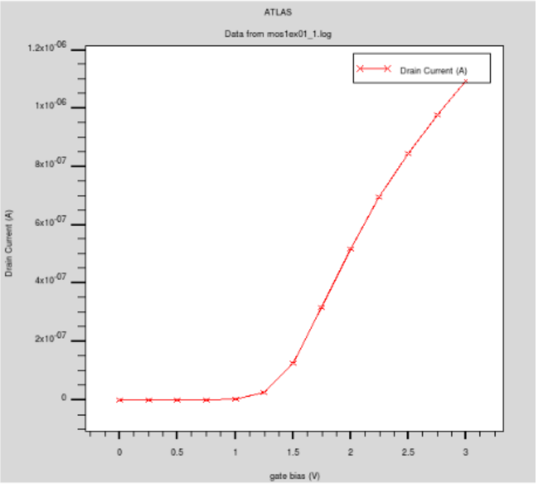

Figure 3. Transfer characteristics of ISFET with 50nm thick nitride film

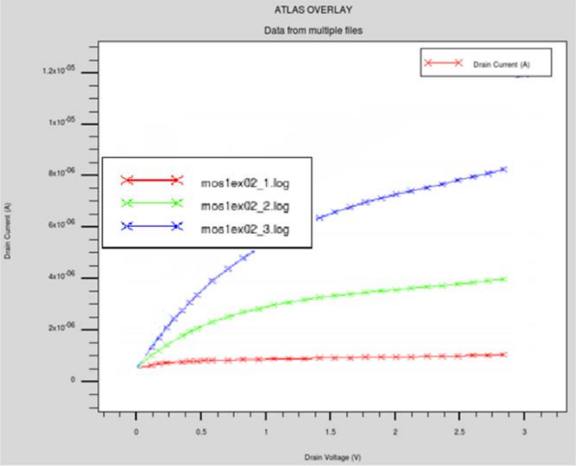

Figure 4. Output characteristics of ISFET with nitride film

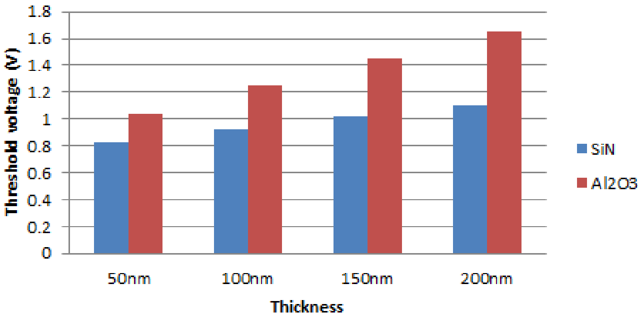

Figure 4. Threshold Voltage Comparison

Figure 4 shows the comparison of Silicon nitride and aluminium oxide sensing films on device performance for various thicknesses. According to the site-binding model, the threshold voltage shift of ISFET is primarily attributed to an interfacial potential at the insulator-electrolyte interface, indicating that the sensitivity depends on the material of the sensing membrane. The threshold voltage changes when the thickness changes. This variation is due to the change in electrochemical parameters such as density on surface sites and dissociation constants. From the results we can conclude that the less thickness, higher the sensitivity.

4. Conclusion

In this paper, we used a model called electrolyte model to simulate the transistor in Silvaco TCAD and analyzed the performance of transistor with silicon nitride and aluminium oxide sensing film for four different thicknesses. According to the operation principle of ISFET, different pH concentrations will induce various surface potentials at the sensing membrane, leading to the variation of threshold voltage.

The threshold voltage of the transistor with silicon nitride sensing film is less than that of the transistor with oxide film. The lower threshold voltage denotes that the transistor is more sensitive. Thus, silicon nitride is the choice for sensing film compared to Aluminum Oxide. When the thickness of the sensing film increases, the threshold voltage also increases. Threshold voltage for four different thicknesses were measured and tabulated. The lower thickness of the sensing film results in higher sensitivity.

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Conflict of interest: The Authors have no conflicts of interest to declare that they are relevant to the content of this article.