TCAD-Based Simulation Method for the Electrolyte–Insulator–Semiconductor Field-Effect Transistor

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Abstract-A simulation method for the electrolyte-insulatorsemiconductor field-effect transistor (EISFET)-type sensor is proposed based on a well-established commercialized semiconductor 3-D technology computer-aided design simulator. The proposed method relies on the fact that an electrolyte can be described using a modified intrinsic semiconductor material because of the similarity between the electrolyte and the intrinsic semiconductor. The electrical double layer of the electrolyte is characterized in the simulation using the Gouy-Chapman-Stern model. Using the proposed simulation method, we extract the Debye lengths depending on phosphate buffered saline solutions with various concentrations and demonstrate that it is possible to simulate the screening effect. Furthermore, we investigate the responses of the EISFET-type silicon nanowire pH sensor based on our simulation method, which shows good agreement with the reported Nernst limit value.

Index Terms—Biosensor, Debye length, electrolyte–insulatorsemiconductor field-effect transistor (EISFET), ion-sensitive field-effect transistor (ISFET), pH sensor, screening effect, silicon nanowire (SiNW), technology computer-aided design (TCAD).

I. INTRODUCTION

PREVIOUSLY, pH values were measured by tracing the voltage produced in glass electrodes. However, glass electrodes are fragile and vulnerable to external stimuli. Moreover, it is difficult to make them smaller and more compact, which inevitably imposes a constraint on their miniaturization, and this is crucial when the pH value in a

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nanosystem is measured. To overcome such issues of glass electrodes, research has been carried out for many years on the electrolyte-insulator-semiconductor field-effect transistor (EISFET), or called ion-sensitive field-effect transistor, as a pH sensor and a biosensor due to its high sensitivity, compactness, ease of use, and low cost [1]. In addition, nanoscale channels in EISFET sensors, such as nanowires and nanotubes, have attracted attention because of their potential use in highly sensitive sensors. Many research groups have attempted to obtain significant experimental results on various types of EISFET-based biosensors [2] and to beat the Nernst limit as well [3]. However, despite these significant technological advances, simulation studies on EISFET sensors have not been well developed and remained insufficient because of the difficulties in simultaneously incorporating both the electrolyte and semiconductor in a simulation. Moreover, a 3-D simulation should be performed when nanoscale EISFET-based sensors, such as nanowire and nanoribbon structures, are considered.

In this brief, we develop a coherent simulation method for the EISFET-type pH sensor using a well-established commercially available 3-D technology computer-aided design (TCAD) [4]. We propose that the electrolyte can be modeled using a modified intrinsic semiconductor because of the similarities between the electrolyte and the semiconductor. In addition, the electrical double layer (EDL), which provides an estimate of the potential distribution in the electrolyte region, is implemented with the Gouy–Chapman–Stern model and the site-binding model (SBM) to describe the electrical characteristics of the electrolyte [5], [6]. We expect that the proposed simulation method will be applicable to detect any of the charged species in field-effect transistor (FET)-based biosensors.

II. SIMULATION METHOD

Because the sensing gate of the EISFET-based sensor is composed of an ionic solution, the implementation of the electrolyte region in the simulation is important [7]. We define the electrolyte region as an intrinsic semiconductor material because the properties of the electrolyte are analogous to those of the intrinsic semiconductor [8]. Both the electrolyte and the intrinsic semiconductor maintain an electrically neutral charge. Moreover, the electrolyte contains many mobile ions, whereas the intrinsic semiconductor contains thermally generated

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electron-hole pairs. In addition, they both are dependent on the Poisson equation and the Boltzmann distribution [9]. However, because the charged particles of the intrinsic semiconductor are electrons and holes that have only one valence, it is impossible to express ions that have more than two valences in the electrolyte in a TCAD simulation. Therefore, the concept of effective ionic concentration $(M_{\rm eff})$ is introduced. The $M_{\rm eff}$ is expressed through the following equation and obtained by calculating the number of ions having a valence that is electrically equal to the ions that have more than two valences [10]:

$$M_{\rm eff} = \frac{1}{2} \sum_{i} c_i z_i^2. \tag{1}$$

Here, *i* is defined as the number of ions in the electrolyte, c_i represents the concentration of the *i*th ion, and z_i indicates the valence of the *i*th ion. For example, in case of $1 \times$ phosphate-buffered saline (PBS), an Meff value of 165.76 mM can be achieved, which is larger than the initial concentration without consideration of ions with two valences. After the $M_{\rm eff}$ value is obtained to describe the electrolyte as the intrinsic semiconductor, the intrinsic carrier density (n_i) is obtained by multiplication of the Avogadro number $(N_A, 6.022 \times 10^{23} \text{ mol}^{-1})$ by the M_{eff} , and then this value is adjusted using the unit of volume (cm^{-3}) to be equal to the $M_{\rm eff}$ as calculated in

$$n_i = M_{\rm eff} \times N_A \times \frac{1}{1000}.$$
 (2)

For the semiconductor, n_i is defined as $(N_C N_V)^{1/2}$ × $\exp(-E_g/2k_BT)$ and is a function of the effective density of states in the conduction band (N_C) and valence band (N_V) , the Boltzmann constant (k_B) , the energy bandgap (E_g) , and the temperature (T). By simply assuming that the effective mass of an electron and a hole are the same, i.e., that N_C is equal to N_V , we can determine the N_C and N_V values for each concentration of PBS at room temperature. For the E_g value, we speculate a small value of 0.1 eV because the calculated n_i value for each concentration of PBS is larger than the n_i value for intrinsic silicon. However, we also obtain the same results when a different value of E_g is employed in the modified intrinsic silicon.

III. RESULTS AND DISCUSSION

To validate the effectiveness of our simulation method, we first extracted the Debye length (λ_D) from the implemented electrolyte in the TCAD simulation to compare the extracted length with the calculated length [7]. The structure of the simulated EISFET-type silicon nanowire (SiNW) sensor is shown in the inset of Fig. 1(a). We introduced a Stern layer with a 0.3-nm thickness for the characterization of the EDL by considering the well-known capacitance of the Stern layer $(C_{\text{Stern}} = 20 \ \mu\text{F/cm}^2)$ and the relative permittivity of the water (6.777) [5], [9]. We intentionally added a positive charge sheet density ($N_0 = 10^{13} \text{ cm}^{-2}$) on the SiO₂ surface to evaluate the potential distribution in the electrolyte. Moreover, it was confirmed that, regardless of the amount of the inserted charge



Diffusion layer potential

Concentration of the PBS

Fig. 1. (a) Simulated potential distribution along the z-direction in relation to various PBS concentrations in the diffusion layer. The inset shows the simulated EISFET-based SiNW sensor structure. We used the SiNW length and width of 1 μ m and 200 nm, respectively. In addition, we used the buried oxide thickness of 145 nm, SiNW thickness of 30 nm, and native oxide thickness of 3 nm. The doping density of the source and drain is 10^{20} cm⁻³ for an n-type, and the doping density of the SiNW channel is 10^{17} cm⁻³ for an n-type (i.e., accumulation mode FET). (b) Comparison between the calculated $\lambda_{D,\text{Cal}}$ [7] and the extracted $\lambda_{D,\text{Ext}}$.

density, the same λ_D can be extracted in each concentration of PBS.

Fig. 1(a) shows the extracted potential distribution in the electrolyte implemented by the proposed modified intrinsic silicon. It should be noted that the capacitance value of the diffusion layer (C_{diff}) has a large value at 1× PBS, while C_{Stern} has a fixed value regardless of the PBS concentration. Therefore, the diffusion layer potential (ψ_d) has a lower value at $1 \times PBS$ than at $0.1 \times$ and $0.01 \times PBS$, as shown in Fig. 1(a). It is also observed that the charges are more quickly neutralized at $1 \times PBS$ because there are more counter ions in $1 \times$ PBS than in 0.01 \times PBS. From these potential distributions in the electrolyte region, we extract the λ_D values in relation to various PBS concentrations. Fig. 1(b) compares the extracted λ_D ($\lambda_{D,Ext}$) with the calculated λ_D ($\lambda_{D,Cal}$). It shows a good agreement within a few percentage points of the errors. Based on the simulation results, we therefore confirm that the electrolyte can be implemented by the modified intrinsic silicon material in the TCAD.

We further simulate the screening effect [7], which is strongly dependent on the concentration of PBS solutions as well, as shown in Fig. 2. The target molecules are designed as a charged sheet layer, as shown in Fig. 2(a). We use the case of streptavidin, and its negative charge density is -2.78×10^{13} cm⁻² [11] in a PBS solution with a pH level of 7.4 [7]. We conduct the simulation by varying the distance (T_{tar}) between the charged sheet layer and the gate dielectric to examine the screening effect.

We observed that I_{DS} decreases at a lower concentration of PBS, as shown in Fig. 2(b), because the C_{diff} of the electrolyte is smaller, and the potential drop is correspondingly larger, at a lower concentration of PBS. For T_{tar} values of 2.3 and 5.0 nm, it is noteworthy that the target molecule does not influence the I_{DS} because the location of the target molecule does not exist within the λ_D , as shown in Fig. 2(c) and (d).

Because we previously confirmed that the electrolyte can be implemented using the modified intrinsic semiconductor, we apply our simulation method to the EISFET-based SiNW



Fig. 2. (a) Schematic of the simulated structure for the screening effect. Here, T_{tar} is the distance between the location of the negatively charged sheet layer and the gate dielectric. At T_{tar} values of (b) 0, (c) 2.3, and (d) 5.0 nm, drain current (I_{DS}) versus liquid-gate voltage (V_{LG}) characteristics are shown according to PBS concentration.



Fig. 3. (a) $I_{\text{DS}}-V_{\text{LG}}$ characteristic for various pH values from 2 to 9 at a V_{DS} of 50 mV. (b) Electrostatic potential according to pH levels ranging from 2 to 9. For the thermal equilibrium state, all electrodes are applied to the ground. (c) Electrostatic potential through the *z*-direction according to the V_{LG} with a step size of -0.2 V.

pH sensor. Fig. 3(a) shows the simulated results of the $I_{\rm DS}-V_{\rm LG}$ characteristics at the drain-to-source voltage ($V_{\rm DS}$) of 50 mV according to various pH values ranging from 2 to 9. In this simulation, we only consider the 0.1 × PBS. The values of surface charge densities on SiO₂ (σ_0) for each pH value on the SiO₂ surface are calculated using the SBM, which has been thoroughly described in [5], [6], and [9]. Because we used a point-of-zero charge of 2.0 on the SiO₂ surface, the calculated values of σ_0 for all of the pH levels have a negative sign [6]. Fig. 3(b) and (c) shows the electrostatic potential through the *z*-direction of the sensor structure for various pH values at a fixed $V_{\rm LG}$ and for various $V_{\rm LG}$ values at a fixed pH value (pH = 7), respectively. Note that the



Fig. 4. (a) Extracted ψ_{eo} in the electrolyte at 0.1× PBS. (b) V_T according to the pH values at 0.1× PBS.

abrupt change in the slope of the potential is shown at the Stern layer due to the negatively charged site-binding layer. We also observed that a positively charged Gouy diffusion layer is formed due to the negatively charged site-binding layer. As the pH value increases, resulting in more negatively charged σ_0 on the site-binding layer, the depletion region is further generated, and the I_{DS} correspondingly decreases for the n-type SiNW, as shown in Fig. 3(a).

Fig. 4(a) shows the potential difference (ψ_{eo}) from the neutral electrolyte to the site-binding layer extracted from Fig. 3(b) for various pH values, which shows that the extracted ψ_{eo} is closely related to the Nernst limit [5]. It is observed that the ψ_{eo} in the electrolyte has a large value in a high pH solution because the value of the intrinsic buffer capacitance is high [7]. It is worth noting that the maximum sensitivity for ψ_{eo} ($\Delta \psi_{eo}$) of 50.3 mV/pH can be achieved between pH 8 and pH 9, as shown in Fig. 4(a), and a good agreement with the Nernst equation is obtained [5]-[7]. The threshold voltage (V_T) for each pH value is extracted, as shown in Fig. 4(b). The extracted ΔV_T values are similar to the $\Delta \psi_{eo}$ values, because the double-layer capacitance (C_{DL}) value is larger than the native oxide capacitance (C_{NOX}) value at $0.1 \times$ PBS [12]. In addition, the simulated ΔV_T shows good consistency with experimental data [5]; therefore, we conclude that our simulation method can be exploited to provide the design and optimization of the EISFET-type sensor.

IV. CONCLUSION

We proposed a simulation method for the EISFET, based on a well-established commercial semiconductor 3-D TCAD simulator. We emulate the electrolyte as an intrinsic semiconductor to simulate the EISFET sensor in TCAD. The effective ionic concentration of the PBS solutions is introduced, and the corresponding n_i is calculated. The λ_D in relation to various concentrations of PBS is extracted and confirmed. The screening effect is also simulated for the verification of the proposed methodology. Using the proposed simulation method, we demonstrate the pH responses of the EISFET-based SiNW pH sensor. Therefore, we expect that our simulation method will provide the theoretical basis of the EISFET-based sensor and enable us to engineer sensor devices.

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