A modified TCAD simulation model for a-InGaZnO based ISFETs on GaAs substrate for pH sensing applications

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Abstract
In this paper, an ISFET model is established and its accuracy is verified. The model can overcome the limitation of TCAD of not supporting electrolyte solution simulation. The source and drain of the model structure are doped with different types of impurities. The influence of GaAs as a substrate on the device sensitivity is also studied. Amorphous indium gallium zinc oxide (a-IGZO) material is used as a semiconductor layer to obtain a new type of ISFET with a higher detection sensitivity to the pH value. Furthermore, the addition of SiC material to the new ISFET further improves the device sensitivity. The influence of different oxide layers on the model when GaAs is used as a substrate is also studied. The results show that the new ISFET can not only break through the Nernst limit of the device sensitivity (59 mV pH⁻¹), but also increase the sensitivity by nearly 12 times.

1. Introduction

During the last few decades, the area of environment and biosensing has been gaining increasing popularity and, therefore, biosensors have been rapidly developed in both research and industry. Since the invention of the ion-sensitive field effect transistor (ISFET) [1] in the 1970s, many researchers have studied the underlying mechanisms of this device model to improve its sensitivity and performance. Mishra et al studied the pH and glucose sensing capabilities of a copper oxide nanosensor based on an EGFET biosensor [2]. The device showed higher sensitivity and linearity than earlier reported pH sensors based on EGFET-based copper oxide nanoparticles [2]. The ISFETs have been widely used in healthcare [3], environmental monitoring [4], food industry [5], biomedicine [6–11] and DNA diagnosis [12].

In order to meet the requirements of digital electronics, researchers have studied and proposed a different structure of ISFET to suppress short channel effects, avoid channel pinch-off, and achieve high current switching ratios. This new type of ISFET is a kind of field-effect element, which has good CMOS process compatibility in the production process [13–15]. Unlike the MOSFET, there are two gates on the top to control the current between the source and drain. The source and drain are doped with different types of impurities and the original silicon substrate is replaced by a layer of oxidation insulators [16–18]. In the future, the ISFET will become a very promising logic device [19].

Nomura et al [20] published a paper in the journal Nature in 2004, and for the first time used amorphous Indium-Gallium-Zinc Oxide (a-IGZO) as a thin film transistor (TFT) channel material to develop a new type of transparent flexible film. The transistor has since opened new avenues in the a-IGZO research. The study found that compared with traditional devices, the a-IGZO TFT has obvious advantages in terms of electron mobility, switching current ratio, sub-threshold coefficient, threshold voltage, and device stability. The excellent performance and high electron mobility of the a-IGZO enhance the sensitivities of the source and drain current of the device to changes in the ionic solubility of the measured solution.

This paper introduces a new type of ISFET structure, where the source and drain are doped with different types of impurities. This structure makes it easier to find the threshold voltage in Silvaco TCAD. As the voltage corresponding to the lowest point of the source and drain current is the threshold voltage, the error is considerably reduced compared with the conventional ISFET having the same type of doping. Moreover, in the
ISFET structure, the substrate is changed to GaAs, and α-IGZO and SiC materials are added, which significantly improves the device sensitivity.

The sensitivity of the back-grid scanning method for the model proposed in [21] is 152.1 mV pH⁻¹. Our model uses GaAs as the substrate, and the sensitivity of the back-grid scanning method can reach a value of 285.0 mV pH⁻¹.

2. Model simulation

To simulate ISFETs in Silvaco TCAD, different solutions should be defined. In this paper, the solution is simplified to the relative permittivity of water [22, 23]. It is assumed that the asymmetric monovalent iron electrolyte is Na⁺, Cl⁻. Considering that the anions/cations in the electrolyte solution and the electrons/holes in the semiconductor have extremely similar characteristics, the ISFET can be simulated in TCAD by regarding the electrolyte as a semiconductor having the dielectric constant of water, i.e., ε = 78 in TCAD [24]. The electron mobility at low temperature is set equal to 6.88 × 10⁻⁴ cm²V⁻¹s⁻¹, which is the value of Cl⁻ ions in water. The hole mobility is set equal to 4.98 × 10⁻⁴ cm²V⁻¹s⁻¹, which is the value of Na⁺ ions in water [25]. In semiconductors, the density of states of the conduction and valence bands, represented by N_C and N_V, respectively, are the most significant correlation parameters between the physical properties of the electrolyte and the intrinsic semiconductor electrical parameters [23]. The electrons and holes can be regarded as freely moving in the electrolyte solution. Therefore, the ion molar concentration of the electrolyte solution can be defined and simulated using N_C and N_V.

Water can be weakly dissociated to a certain extent, and its ionization equation is as follows [23]:

\[ H_2O \leftrightarrow K_w H^+ + OH^- \]  (1)

where \( K_w \) is the dissociation constant of water, defined as

\[ K_w = [H^+][OH^-] \]  (2)

Under standard pressure and temperature conditions, \( K_w \) is equal to 10⁻¹⁴ times the ion concentration.

The ISFET is sensitive to ions because the electrolyte solution reacts with the insulator on its surface to generate surface charges. This reaction can be described by the adsorption bonding model theory [26] as shown by the following expression [32]:

\[ \sigma_0 = qN_{fl} \left( \frac{p n_i^2 - K_a K_b n}{p n_i^2 + K_a K_b n + K_b n_i^2} \right) \]  (3)

In (3), \( \sigma_0 \) is the surface charge density, \( n \) is the electron concentration, \( p \) is the hole concentration, \( q \) is the basic charge, \( N_{fl} \) is the number of amphoteric sites with both positive and negative charges per unit area, and \( K_a \) and \( K_b \) are the dissociation constants of the insulator. The intrinsic carrier concentration is given by \( n_i \). As the electrons (holes) are regarded as ions, \( n_i \) is expressed as 6.022 × 10¹³ [27]. When the material is SiO₂, the values of \( N_{fl} \) is \( K_a \) and \( K_b \) are \( 5 \times 10^{14} \) and \( 10^{10} \), respectively [28].

As polycrystalline IGZO is a disordered material, the band gap contains a large number of defective state densities and, therefore, modeling is needed to simulate the defect state distribution. Here, the properties of the intermediate gap state density of amorphous silicon (a-Si) [29] are used. The density of different defective states is represented as follows [30]:

\[
\begin{align*}
\gamma_{TA}(E) &= N_{TA} \exp \left[ \frac{E - E_C}{W_{TA}} \right] \\
\gamma_{TD}(E) &= N_{TD} \exp \left[ \frac{E_V - E}{W_{TD}} \right] \\
\gamma_{GD}(E) &= N_{GD} \exp \left[ \frac{E - E_{GD}}{W_{GD}} \right] 
\end{align*}
\]  (4)

In (4), \( E \) is the trap energy level, \( E_C \) is the conduction band bottom energy level, \( E_V \) is the valence band top energy level. \( \gamma_{TA}(E) \) is the exponential density of the acceptor-like subgap states, \( \gamma_{TD}(E) \) is the exponential density of donor-like subgap states, and \( \gamma_{GD}(E) \) is the Gaussian density of donor-like states (oxygen vacancies).

According to [30], \( N_{TA}, N_{TD}, W_{TA}, W_{TD}, N_{GD}, E_{GD} \) and \( W_{GD} \) are the relevant parameters of α-IGZO that are described and assigned in table 1.

Based on the experimental report of Mohammadi and Manavizadeh published in 2019 [21], the following conclusions can be obtained: Unlike traditional ISFETs, when a voltage is applied to the fluid gate, the device is always on. A strong inversion layer will form under the gate when the fluid gate voltage increases, forming a
p-n-n structure from the drain to the source. A reduction in the fluid gate voltage will form a p-p-n structure. In the new ISFET, \( V_{th} \) can be determined by finding the lowest current when analyzing the transfer characteristics of the new ion sensitive device, which reduces the experimental error. In order to reduce these errors, a specific modeling of the electric double layer–Stern layer generated by the plane reaction is carried out. Using the known Stern layer capacitance \( (C_{stern} = 20 \ \text{\mu F/cm}^2) \) [31], the Stern layer is simulated as a semiconductor with a dielectric constant to adapt it to the model. A new ISFET structure is formed by doping the source and drain of the model structure with different types of impurities having the same concentration, as shown in figure 1.

A new ISFET structure is formed by doping the source and drain of the model structure with different types of impurities having the same concentration, as shown in figure 1. The solution layer has a length of 30 nm and a thickness of 12 nm. The length of the Stern layer is 30 nm and its thickness is 1 nm. The length of the insulating layer is 30 nm and its thickness is 5 nm. In figure 1, SiO₂ is used as the insulating layer. The Si layer has a length of 40 nm and a thickness of 20 nm. The length and thickness of the Buried Oxide layer are 40 nm and 50 nm, respectively, while the length and thickness of the GaAs layer are 40 nm and 70 nm, respectively.

### 3. Simulations and analysis

#### 3.1. Ion-sensitive field effect transistor with GaAs substrate

The change of pH value will change the concentration of carriers in the channel, thereby changing the p-n junction characteristics and the current between the drain and the source. Different pH values will correspond to different \( V_{th} \) values. Thus, we can calculate the sensitivity of the device by detecting the change in \( V_{th} \).

The sensitivity of the device is defined as follows:

\[
\text{Sensitivity} = \frac{V_{th}(PH_2) - V_{th}(PH_1)}{PH_2 - PH_1}
\]

In the simulations, the source is grounded, \( V_{DS} \) is set to 400 mV, and the fluid gate voltage is scanned. In Silvaco TCAD, the ISFET uses electrolyte solution instead of the MOSFET gate. The sensitivity of the device with SiO₂ as the insulating layer is tested with pH values ranging from 4 to 8 in order to verify the model accuracy, as shown in figure 2. It can be observed that increasing the pH value can increase the threshold voltage and shift the overall trend to the right.

The sensitivity of the device with SiO₂ as the insulating layer is 59.5 mV pH⁻¹, which is consistent with the theoretical limit (59 mV pH⁻¹) of Nernst, thus validating the accuracy of the model in Silvaco TCAD. In order to further improve the sensitivity of ISFET, experiments are carried out by scanning the back gate voltage. It can be seen from figure 2 that this method has a trend similar to the I-V characteristics obtained by scanning the fluid gate voltage. However, since the back gate dielectric layer is thicker than the insulating layer, a higher voltage needs to be applied to the back gate to form a strong inversion layer in the channel. Therefore, the trend of I-V characteristics is enlarged, and the corresponding sensitivity is improved, as shown in figure 3. The results in figure 3 show that the device sensitivity reaches 285.0 mV pH⁻¹.

#### 3.2. Ion-sensitive field effect transistor with GaAs substrate and a-IGZO material

Based on the above source and drain doping with different types and uniform concentrations of impurities, the ISFET structure is formed by adding a-IGZO, which has excellent performance and higher electron mobility. These characteristics can improve the sensitivity of the source leakage current of the device to changes in the ion

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**Table 1. Relevant parameters of a-IGZO used in simulations.**

| Parameter                                      | a-IGZO [30] |
|-----------------------------------------------|-------------|
| Electron affinity \( (\chi) \) (eV)          | 4.16        |
| Band gap \( (E_g) \) (eV)                     | 3.05        |
| Mobility of electrons \( (\mu_n) \) (cm² V⁻¹ s⁻¹) | 15          |
| Mobility of holes \( (\mu_p) \) (cm² V⁻¹ s⁻¹)  | 0.1         |
| Effective density of states in conduction band \( (N_{c}) \) (cm⁻³) | \( 5 \times 10^{14} \) |
| Effective density of states in valence band \( (N_{v}) \) (cm⁻³) | \( 5 \times 10^{14} \) |
| Densities of acceptor-like tail state \( (N_{TA}) \) (cm⁻³ eV⁻¹) | \( 1.55 \times 10^{20} \) |
| Densities of donor-like tail states \( (N_{TD}) \) (cm⁻³ eV⁻¹) | \( 1.55 \times 10^{20} \) |
| Characteristic decay energy in the conduction band tail states \( (W_{c}) \) (eV) | 0.013 |
| Characteristic decay energy in the valence band tail states \( (W_{v}) \) (eV) | 0.12 |
| Peak value of the density of donor-like states in the Gaussian distribution \( (N_{GD}) \) (cm⁻³ eV⁻¹) | \( 6.5 \times 10^{16} \) |
| Central energy \( (E_{GD}) \) (eV) | 2.9 |
| Characteristic decay energy \( (W_{GD}) \) (eV) | 0.1 |
Figure 1. Structure diagram of the new ISFET.

Figure 2. (a) I-V characteristics and the corresponding sensitivity of fluid gate voltage versus source-drain current at different pH values. (b) $V_{th}$ and the corresponding sensitivity at different pH values in (a).

Figure 3. (a) I-V characteristics and the corresponding sensitivity of back gate voltage versus source-drain current at different pH values. (b) $V_{th}$ and the corresponding sensitivity at different pH values in (a).
solubility of the measured solution. The length and thickness of the a-IGZO layer are 40 nm and 30 nm, respectively. Figure 4 shows the device structure.

Table 1 shows the parameters of a-IGZO material used for modeling the structure in TCAD.

The simulations use GaAs as the substrate, and tests the sensitivity of the device using SiO₂ as the insulating layer, with pH values ranging from 4 to 8, as shown in Figure 5. The results show that the sensitivity of the device is 351.1 mV pH⁻¹, which increases by about 70 mV pH⁻¹ compared to the case when GaAs are used as the substrate.
Figure 6. (a) I-V characteristics of the back gate voltage versus source-drain current of the ISFET with Si$_3$N$_4$ as the insulating layer and GaAs as the substrate. (b) $V_{th}$ and the corresponding sensitivity under different pH values in (a). (c) I-V characteristics of back gate voltage versus source-drain current of ISFET with Al$_2$O$_3$ as the insulating layer and GaAs as the substrate (d) $V_{th}$ and the corresponding sensitivity under different pH values in (c). (e) I-V characteristics of back-gate voltage versus source-drain current of ISFET with Ta$_2$O$_5$ as the insulating layer and GaAs as the substrate (f) $V_{th}$ and the corresponding sensitivity under different pH values in (e).
3.3. Influence of different insulating layers on device sensitivity

The influence of insulating materials on device sensitivity is studied by using Si$_3$N$_4$, Al$_2$O$_3$, and Ta$_2$O$_5$ as insulating layer materials. Table 2 shows the relevant parameters of different insulating layers [28].

Figure 6 shows the I-V characteristics and sensitivity values of the back-gate voltage and source-drain current of ISFETs with different insulating layers.

The results show that the sensitivity values of ISFET with SiO$_2$, Si$_3$N$_4$, Al$_2$O$_3$ and Ta$_2$O$_5$ as the insulating layers are equal to 351.1 mV pH$^{-1}$, 458.8 mV pH$^{-1}$, 552.9 mV pH$^{-1}$ and 585.3 mV pH$^{-1}$, respectively.

3.4. Ion-sensitive field effect transistor with SiC material

The SiC material has the characteristics of wide band gap, high critical breakdown electric field, high thermal conductivity, high carrier saturation drift speed, etc. The length and thickness of the SiC layer are 40 nm and 50 nm, respectively. Figure 7 shows the device structure.

Therefore, it is added to the new ISFET, and the sensitivity of the device that uses SiO$_2$ as the insulating layer is tested with pH values ranging from 4 to 8, as shown in figure 8. The results show that the sensitivity of the device is 432.5 mV pH$^{-1}$, which improves by about 81 mV pH$^{-1}$ compared with the case where SiC material is not added and SiO$_2$ is used as the insulating layer.
The influence of different insulating materials on the sensitivity of a device containing SiC is tested by using Si$_3$N$_4$, Al$_2$O$_3$, and Ta$_2$O$_5$ as the insulating layer materials. Figure 9 shows the results.

The results show that the sensitivity values of ISFET with SiC as the insulating layer, under different pH values, are equal to 567.5 mV pH$^{-1}$, 682.5 mV pH$^{-1}$, and 695.1 mV pH$^{-1}$, respectively. For the model proposed in [21], the sensitivity of back-grid scanning method is 152.1 mV pH$^{-1}$. Our model uses GaAs as the substrate, and the back-grid scanning method can reach achieve a sensitivity of 285.0 mV pH$^{-1}$. In addition, a-IGZO material is added, which improves the sensitivity to 285.0 mV pH$^{-1}$. The sensitivity is
further increased to 432.5 mV pH$^{-1}$ by adding the SiC material to the model. The insulating layer material SiO$_2$ is replaced by Ta$_2$O$_5$, and as a result the sensitivity reaches a value of 695.1 mV pH$^{-1}$.

4. Conclusion

This article introduced a new type of ISFET and the effect of using GaAs as a substrate on the sensitivity of the device was studied. In addition, the analysis method of scanning the back gate voltage could amplify the I-V trend of the ISFET, thereby increasing the sensitivity to three times the Nernst limit. In addition, a-IGZO material was added to amplify the I-V trend of ISFETs to further increase the sensitivity to four and a half times the Nernst limit. The addition of SiC materials further amplified the I-V trend of ISFETs to increase the sensitivity to seven times the Nernst limit. This paper also studied the influence of different insulating layer materials on the sensitivity of the device. The results showed that when Ta$_2$O$_5$ and GaAs were used as insulating materials and substrates, the highest sensitivity of ISFET with SiC added was 695.1 mV pH$^{-1}$. The results showed that the new ISFET could break through the Nernst limit of device sensitivity (59 mV pH$^{-1}$), and the sensitivity could reach nearly 12 times the Nernst limit.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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References

[1] Bergveld P 1970 Development of an ionsensitive solid state device for neurophysical measurements IEEE Trans. Biomed. Eng. 17 70–1
[2] Mishra A K, Jarwal D K, Mukherjee B, Kumar A, Ratan S and Jit S 2020 CuO Nanowire-based extended-gate field-effect-transistor (FET) for pH sensing and enzyme-free–receptor-free glucose sensing applications IEEE Sens. J. 20 5039–47
[3] Jimenez-Jorquera C, Orozco J and Baldi A 2009 ISFET based microsensors for environmental monitoring Sensors 10 61–83
[4] Nakata S, Arie T, Akita S and Takei K 2017 Wearable, flexible, and multifunctional healthcare device with an ISFET chemical sensor for simultaneous sweat pH and skin temperature monitoring ACS Sensors 2 443–8
[5] Mu L, Chang Y, Sawtelle S D, Wipf PM, Duan X and Reed M A 2015 Silicon nanowire field-effect transistors—a versatile class of potentiometric nanobiosensors IEEE Access 3 287–302
[6] Nair P R and Alam M A 2007 Design considerations of silicon nanowire biosensors IEEE Trans. Electron Devices 54 3400–8
[7] Wu T, Alharbi A, Y ou K-D, Kisslinger K, Stach E A and Shahrjerdi D 2017 Experimental study of the detection limit in dual-gate biosensors using ultrathin silicon transistors ACS Nano 11 7142–7
[8] Hajmizadehsharif M et al 2016 Ultra-high sensitivity DNA detection using nanorods incorporated ISFETs IEEE Electron Device Lett. 37 663–6
[9] Mahdavi M, Samaean A, Hajmizadehsharif M, Shahmohammadi-M hadi, M, Mohajerzadeh S and Malboobi M A 2014 Label-free detection of DNA hybridization using a porous poly-Si ion-sensitive field-effect transistor RSC Adv. 4 46854–63
[10] Zeng R, Zhang J, Sun C, Xu M, Zhang S-L and Wu D 2018 A referenceless semiconductor ion sensor Sens. Actuators B, Chem. 254 102–9
[11] Moser N, Lande T S, Toumazou C and Georgiou P 2016 ISFETs in CMOS and emergent trends in instrumentation: a review IEEE Sensors J. 16 6496–514
[12] Cacho-Soblechero M, Malpartida-Cardenas K, Ciaciello C, Rodriguez-Manzano J and Georgiou P 2020 A dual-sensing thermo-chemical ISFET array for DNA-based diagnostics IEEE Transactions on Biomedical Circuits and Systems 14 477–89
[13] Amirmazlaghani M and Raissi F 2009 Memory cell using modified field effect diode IEICE-E Commun. Express 6 1582–6
[14] Cao S et al 2010 Design and characterization of ESD protection devices for high-speed I–O in advanced SOI technology IEEE Transactions on Electron Devices 57 644–53
[15] Jafari Touchaei B and Manavizadeh N 2015 An inverter gate design based on nanoscale S–FED as a function of reservoir thickness IEEE Trans. Electron Devices 62 5147–52
[16] Sheikhan I and Raissi F 2007 Simulation results for nanoscale field effect diode IEEE Trans- actions on Electron Devices 54 613–7
[17] Kato N et al 2017 An AlGaN/GaN field effect diode with a high turn-on voltage controllability Physica Status Solidi A Applications & Materials Science 214 600830
[18] Vadzaihe M 2016 Improving gate delay and $I_{ON}/I_{OFF}$ in nanoscale heterostructure field effect diode (H–FED) by using heavy doped layers in the channel Applied Physics A, Materials Science & Processing 122 469
[19] Touchaei B J and Manavizadeh N 2016 Design and simulation of low-power logic gates B–used on nan-oscale side-contacted FED IEEE Trans. Electron Devices 99 1–6
[20] Nomura K et al 2004 Room–temperature fabrication of transparent flexible thin-film transistors using amorphous oxide semiconductors Nature 432 488–92
[21] Mohammadi E and Manavizadeh N 2019 Performance evaluation of innovative ion-sensitive field effect diode for pH Sensing IEEE Sens. J. 19 1239–44
[22] Wu T, Alharbi A, You K-D, Kisslinger K, Stach E A and Shahrjerdi D 2017 Experimental study of the detection limit in dual-gate biosensors using ultrathin silicon transistors ACS Nano 11 7142–7
[23] Jang H-J and Cho W-J 2014 Performance enhancement of capacitive-coupling dual-gate ion-sensitive field-effect transistor in ultra-thin-body Sci. Rep. 4 5284-1–5284-8
[24] Narang R, Saxena M and Gupta M 2017 Analytical model of pH sensing characteristics of junctionless silicon on insulator ISFET IEEE Trans. Electron Devices 4 1–9
[25] Koneshan S et al 1998 Solvent structure, dynamics, and ion mobility in aqueous solutions at 25 °C J. phys. chem. b 102 4193–204
[26] Yates D E, Levine S and Healy T W 1974 Site-binding model of the electrical double layer at the oxide/water interface J. Chem. Soc. Faraday Trans. 70 1807–18
[27] Daniele P et al 2015 Numerical simulation of ISFET structures for biosensing devices with TCAD tools Biomed. Eng. Online 14 53
[28] Bandiziol A, Palestri P, Pintino F, Esseni D and Selmi L 2015 A TCAD-based methodology to model the site-binding charge at ISFET/electrolyte interfaces IEEE Trans. Electron Devices 62 3379–86
[29] Fung T C et al 2009 Two-dimensional numerical simulation of radio frequency sputter a-morphous In-Ga-Zn-O thin-film transistors J. Appl. Phys. 106 84511
[30] Narendra K et al 2020 Interface mechanisms involved in a-IGZO based dual gate ISFET pH sensor using Al2O3 as the top gate dielectric Mater. Sci. Semicond. Process. 119 105239
[31] van Hal R E G, Eijkel J C T and Bergveld P 1996 A general model to describe the electrostatic potential at electrolyte oxide interfaces Adv. Colloid Interface Sci. 69 31–62
[32] Mohammadi E and Manavizadeh N 2018 An accurate TCAD-based model for ISFET simulation IEEE Transactions on Electron Devices 65 (IEEE) pp 3950–6