



Performance optimization of single-layer and double-layer high-k gate nanoscale ion-sensitive field-effect transistors

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ABSTRACT

The use of high-k dielectric materials for the gate insulator of nanoscale Ion-Sensitive Field-Effect Transistor (ISFET) has been demonstrated to generally improve the ISFET performance. High-k gate insulator reduces the gate leakage current and increases the gate capacitance, which lead to higher *trans*-conductance and higher current sensitivity. The best high-k material for ISFET sensors is not simply the material of highest dielectric constant because high-k ISFET performance depends on many conflicting factors such as dissociation properties with electrolytes and linearity of voltage/current variation with pH change. In this work, a comparative simulation study is presented for six high-k gate insulators (Si_3N_4 , Al_2O_3 , ZrO_2 , Ta_2O_5 , HfO_2 , and TiO_2), along with SiO_2 for comparison, for nanoscale ISFET sensors, comparing their sensitivity and linearity. The simulation tool used (NIST) is based on the numerical solution of nanoscale ballistic MOSFET equations along with Gouy-Chapman-Stern model equations. The study presents a guideline for the determination of the optimum insulator material and insulator thickness used for nanoscale ISFETs. The study included single-layer as well as double-layer insulators in which two layers of different dielectric materials are used.

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1. Introduction

Ion-Sensitive Field-Effect Transistor (ISFET) first introduced by Bergveld in 1970 [1] is now one of the promising structures, which has attracted much attention for many sensing applications such as agriculture, environmental monitoring, food industry, as well as lab-on-chip and health-care applications [2]. Although it was originally developed for pH sensing, it has subsequently been used for electronic detection of various types of biomolecules [3]. ISFET sensors offer advantages of low cost, label-free detection, and being potentially suitable for massive parallelization [4]. Moreover, they can be produced using standard CMOS technology and may have miniaturized that make them feasible for use with micro/nano-systems [5].

ISFET sensitivity can be measured using two approaches: the first is to use a fixed value for the reference electrode voltage, V_{ref} and to take the change in drain current I_D per unit pH change, S_1 , as ISFET sensitivity. Alternatively, the second method is to use a readout circuit to maintain the drain current at a predefined value

and to take the required V_{ref} shift per pH change as a measure of device sensitivity. Here, the sensitivity is the change in V_{ref} per pH unit change, denoted by S_2 [6]. S_1 and S_2 are called current and voltage sensitivities of ISFET, respectively.

Aiming to satisfy extensively miniaturized, low-cost ISFETs, the device dimensions may reach the nanoscale range in which the gate insulator thickness is few nanometers. This leads to a high leakage gate current and make it more vulnerable to dielectric breakdown. One of the solutions of this problem is the use of high-k dielectric materials for the gate insulator [7]. This has been demonstrated to generally improve the ISFET performance [8–10]. High-k gate materials enable the use of thicker gate insulators which diminishes the gate leakage current [8]. It also increases the gate capacitance which leads to the increase of the *trans*-conductance of the device as well as the ISFET current sensitivity. Moreover, High-k dielectrics reduce current instability by lowering destabilizing ion transport within passivation layer due to contact with fluids [4]. The use of high-k dielectric ISFETs with good liquid gate transfer characteristics paves the way towards integrated sensing circuits [8].

Many types of dielectrics were adopted as high-k gate insulator in ISFET, such as, Silicon Nitride Si_3N_4 [5,11–13], Aluminum oxide Al_2O_3 [5,13–15], Zirconium dioxide ZrO_2 [16], Tantalum oxide Ta_2O_5 [9,13,17,18], Titanium dioxide TiO_2 [10], Hafnium dioxide HfO_2 [4,8,17,19], and Praseodymium oxide Pr_2O_3 [20]. Many of

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the pervious investigations of high- k gated ISFETs used experimental characterization while few of them used numerical simulation [5,11,13,18]. Some of the studies investigated the effect of stacking two dielectric layers on the ISFET sensitivity [12,19]. For each of the above studies, the focus was on some specific individual types of dielectrics.

This work presents a simulation study for single-layer and double-layer gate insulators of ISFET pH sensor. Six high- k insulator types are taken into consideration: Si_3N_4 , Al_2O_3 , ZrO_2 , Ta_2O_5 , HfO_2 , and TiO_2 along with SiO_2 for comparison. The effect of dielectric type, its thickness, and biasing conditions on the ISFET performance are explored. The simulation tool used is called NIST (Numerical ISFET Simulation Tool) [5], which is based on the numerical solution of nanoscale ballistic MOSFET equations along with Gouy-Chapman-Stern model equations. For the underlying MOSFET physics, previous modelling methods depend on either closed form analytical equations [21–23], using foundry specific SPICE model [24], or post processing using commercially available TCAD software of conventional MOSFET [2,25]. Alternatively, a ballistic transport numerical model is used here using NIST software tool [5]. The study gives a guideline for the determination of the suitable value of fixed reference voltage, V_{ref} and drain current, I_D that can be used to measure pH value. It also presents a figure of merit for the optimization of the sensor performance based on two factors: the first is the maximization of the average sensitivity along the pH range, and the second is the minimization of the variability of sensor sensitivity with pH change, which is measured by the standard deviation of sensitivity with pH. Since ballistic nanoscale ISFETs have the advantage of small size, large current levels, simulation of such ISFETs enables the exploitation of these advantages.

Section 2 reviews the simulation method used to calculate ISFET output current for a certain value of solution pH. The results are presented and discussed in Section 3 for both single layer and double layer structures. In Section 4, the conclusions of the study are summarized.

2. Simulation method

ISFET simulation is performed using Nanoscale ISFET Simulation Tool (NIST) developed in [5]. The underlying theory, main building blocks, and mathematical equations of this tool are described hereinafter. The ISFET structure depicted in Fig. 1 can be divided into two main parts: the first part is the MOSFET structure which consists of the gate insulator and the underlying channel connecting source

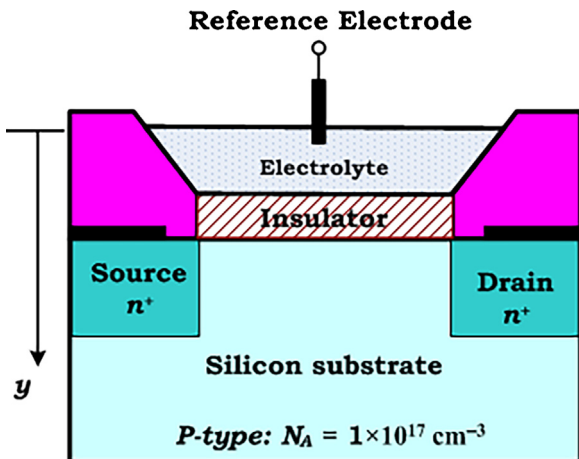


Fig. 1. A schematic diagram of a nanoscale ISFET in which the gate insulator can be made of one layer or two layers of different materials.

and drain terminals, and the second part is the electrolyte for which pH is measured with a reference electrode immersed in the electrolyte. The two parts are interacting through the electrolyte-gate insulator interface. The pH of the electrolyte will determine the amount of charge induced on the electrolyte-insulator interface, σ_i , which changes the potential of this interface, ψ_i . This potential plays the role of gate voltage in conventional MOSFETs. Thus, the electrostatics of the underlying MOSFET structure can be described by nanoscale ballistic MOSFET theory [26], based on two main equations: the first equation relates the charge density in the channel σ_{MOS} to the surface potential in the channel ψ_s :

$$\sigma_{MOS} = \frac{qk_B T}{2} g_{2D} \{ \log [1 + e^{\eta_{FS}}] + \log [1 + e^{\eta_{FD}}] \} \quad (1a)$$

where q is the electronic charge, k_B is the Boltzmann constant, T is the temperature, $g_{2D} = (2m^*/\pi\hbar^2)$ is the silicon 2D density of states including spin and valley degeneracy, m^* is the electron effective mass, \hbar is the modified Planck's constant, η_{FS} and η_{FD} are defined as

$$\eta_{FS} = (E_{FS} + q\psi_s)/k_B T \quad (1b)$$

$$\eta_{FD} = (E_{FD} + q\psi_s)/k_B T \quad (1c)$$

with E_{FS} and $E_{FD} = E_{FS} - qV_D$ are the quasi-Fermi levels at source and drain, respectively, for a drain-to-source voltage V_D .

The second equation models the device electrostatics using three model capacitances: C_G , C_D , and C_S representing channel-to-gate, channel-to-drain, and channel-to-source capacitances per unit area, respectively, which can be written as,

$$\psi_s = \alpha_G \psi_i + \alpha_D V_D + (\sigma_{MOS} - \sigma_o)/C_{tot} \quad (2)$$

with $C_{tot} = C_G + C_D + C_S$ is the sum of the three model capacitances, $\alpha_G = C_G/C_{tot}$, $\alpha_D = C_D/C_{tot}$, and σ_o is the charge density at zero bias [5]. ψ_i is put here in place of gate voltage used in conventional MOSFETs.

On the other side, the charge electrostatics of the electrolyte and the electrolyte-insulator interface can be described using Gouy-Chapman-Stern theory [21,27] and some accompanying electrostatic equations, recalled here for clarity as follows [2,5],

$$\sigma_{MOS} + \sigma_i + \sigma_d = 0 \quad (3)$$

Eq. (3) represents the condition of charge neutrality for the whole system, where σ_{MOS} is the surface charge density in the semiconductor channel, σ_i is the surface charge density on the insulator-electrolyte interface resulting from ion adsorption, and σ_d is the continuous charge density distribution through the diffuse layer. For the Helmholtz layer, σ_d is related to the potential at the edge of diffuse layer, ψ_d , and the electrolyte-insulator interface potential through,

$$\sigma_d = C_h (\psi_d - \psi_i) \quad (4)$$

where C_h is the capacitance of the Helmholtz layer, and for the Gouy-Chapman layer,

$$\sigma_d = \sqrt{8\varepsilon_o \varepsilon_{rw} k_B T c_0} \sinh \left(\frac{q(V_{ref} - \psi_d)}{2k_B T} \right) \quad (5)$$

ε_{rw} is the relative dielectric constant of water, ε_o is the free-space permittivity, c_0 is the solution ion concentration, and V_{ref} is the reference voltage. The surface charge density on the insulator-electrolyte interface is

$$\sigma_i = qN_{sil} \left(\frac{[\text{H}^+]_s^2 - K_+ K_-}{[\text{H}^+]_s^2 + K_+ [\text{H}^+]_s + K_+ K_-} \right) + qN_{nit} \left(\frac{[\text{H}^+]_s}{[\text{H}^+]_s + K_{N+}} \right) \quad (6)$$

where N_{sil} and N_{nit} are number of silanol sites and primary amine sites per unit area, respectively; K_+ , K_- , and K_{N+} are the dissociation

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