PARAMETER EXTRACTION FOR ELECTRO-CHEMICAL SIMULATIONS OF ION SENSITIVE TRANSISTORS

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ABSTRACT: Proper CAD design of electronic microsystems oriented for environment monitoring requires accurate models of various ambient sensors. In particular, this paper presents a simple but accurate model of the ion sensitive transistor. The model parameters are determined based on electrical measurements of a real ion sensitive transistor. The measurement results are compared with SPICE simulations and discussed.

INTRODUCTION

Modern electronic microsystems comprise various devices operating based on different phenomena not necessarily purely electrical ones. Therefore, electronic system engineers need some adequate simulation tools rendering possible multidomain simulation of such microsystems. Sometimes it is possible to simulate these devices in electrical simulators by simply adapting existing device models. This approach was employed by the authors for SPICE simulations of an Ion Sensitive Field Effect Transistor (ISFET). These transistors are necessary in water pollution monitoring applications where they can serve, depending on the chosen gate membrane, as detectors for different ions.

The next section of the paper provides some theoretical background on the ISFET operation principle and its electro-chemical model used by the authors in the simulations. Then, the results of electrical measurements obtained for several ISFETs are presented in detail. Next, based on the measurements, the model parameter extraction is performed. Finally, the simulation results are compared with the measurements and discussed.

ISFET MODELLING

Operation principle

Essentially, the Ion Sensitive Field Effect Transistor (ISFET) is a Metal Oxide Semiconductor FET (MOSFET) in which the standard metal- polysilicon gate is replaced by a more complex structure sensitive to hydrogen ion concentration. The gate structure, presented in Figure 1, consists of a reference electrode and an insulating material between which a measured electrolyte flows. The electrolyte closes the electric gate-source circuit and the ion concentration influences the gate potential which in turn modifies the transistor threshold voltage In such a way the hydrogen ion concentration can exercise electrostatic control on the drain-source current.

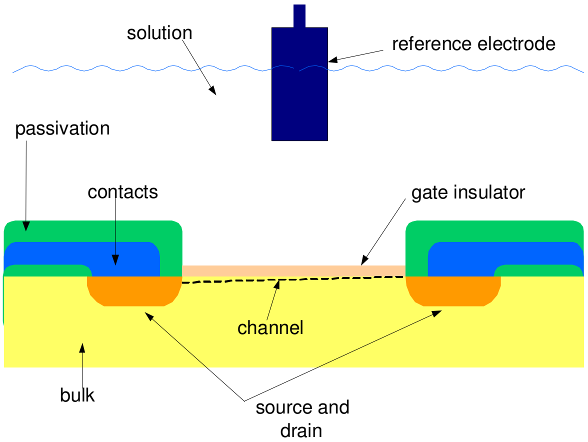

Figure 1: Cross-section of an ISFET structure

The ISFETs are usually operated in the constant 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 modification of the reference electrode potential (the gate voltage).

Therefore, the sensitivity of an ISFET is usually expressed as the gate voltage change per decade of the hydrogen ion concentration pH, where the pH denotes $-\log [H^+]$. For example, if the value of the pH is equal to 2, the concentration of the hydrogen ions amounts to 10^{-2} mole per liter.

The ISFET sensitivity depends mainly on the choice of the gate insulator material. The most commonly used materials are silicon and metal oxides or nitrides. Among these materials, especially high sensitivity to the hydrogen ion concentration exhibits the aluminium oxide.

Additionally, when the gate is coated with a special membrane, an ISFETs can be used for the detection of various species in the surrounding electrolyte, other than the hydrogen ions. Such a transistor with some ion selective membrane and the so-called PolyHEMA layer stabilising the operation of the sensor is known as the CHEmically Modified Field Effect Transistor (CHEMFET).

Electrochemical model

The operation of an ISFET sensor can be explained by the so-called site-binding theory [1-2]. The theory assumes that potential of the solid-liquid interface, gate insulator–electrolyte in the considered case, depends mainly on the concentration of the hydrogen ions in the analysed solution. The ions from the solution react with the active sites of the insulator. The process of the "hydrogen – active site" pairs creation changes the total value of the charge of the active sites on the insulator surface hence influencing the transistor channel current. Additionally, some other ions present in the solution might react with the insulator active sites and influence the sensor operation. These ions are called disturbing anions or cations.

According to the Gouy-Chapman–Stern theory [3-4] a double layer is created at the insulator-electrolyte border as shown in Figure 2. The double layer consists of the diffuse layer and the Helmholtz layer. In the considered case, the Helmholtz layer comprises the layer of the adsorbed hydrogen ions and the common plane of the adsorbed disturbing anions and cations.

The electrical representation of the double layer is also shown in Figure 2. The letters *C*, σ and ψ denote capacitance, charge and potential respectively. The indexes *D, AK, S, C* and *ins* refer to the diffusion layer, disturbing ions, the insulator surface, the transistor channel and the insulator respectively. Based on the theory, a system of non-linear equations can be created. The system of equations allows the computation of the surface potential ψ_s dependence on the hydrogen ion concentration pH. The obtained theoretical solution, which turns out to be almost a straight line, is presented in Figure 3. The computed values of the potential will be used later to modify the transistor threshold voltage in the SPICE model presented in the next subsection. More detailed considerations on the theory of the ISFET electro-chemical model can be found in [5]

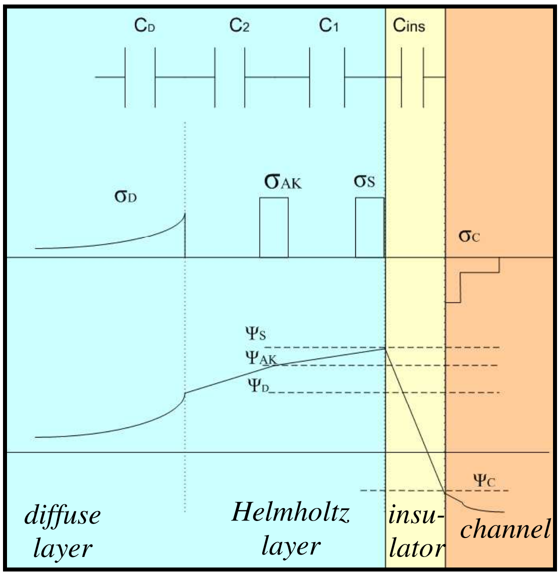

Figure 2: Charge and potential distribution in solid-liquid interface and electrical model of the double layer

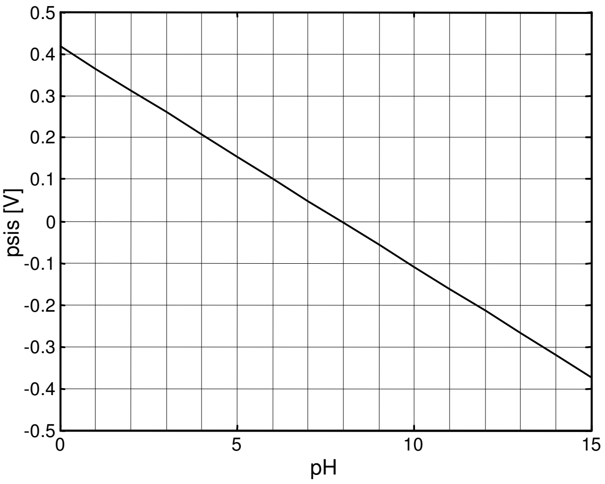

Figure 3: Theoretical dependence of insulator surface potential on hydrogen ion concentration

SPICE Model

For the electrical simulations, the authors adapted the existing SPICE MOSFET model, in which the threshold voltage is chemically modified through the surface potential. This approach is not entirely new and was proposed already in the early nineties, e.g. in [6].

The preliminary simulations demonstrated that the first level of the SPICE model was not accurate enough. Thus, for the actual simulations a simplified version of the third level SPICE model was employed. The fact that the transistor under consideration was wide and long allowed the simplification of the model by neglecting in the model most of the short channel terms. Thus, the transistor output characteristics can be described by the following equation:

$$I_D = \frac{C_{ox}\,\mu_{eff}}{2}\,\frac{W_{eff}}{L_{eff}}\,(2\,(V_{GS} - V_T) - V_{DS})\,V_{DS} \quad (1)$$

where:
I_D *– transistor drain current*
C_{ox} *– gate dielectric capacitance per unit area*
μ_{eff} *– effective carrier mobility*
W_{eff}, L_{eff} *– effective channel width and length*
V_{DS}, V_{GS} *– drain-source and gate-source voltages*
V_T *– transistor threshold voltage*

The major difference between the adopted model and the simple Level 1 SPICE model is the introduction of variable carrier mobility in the channel. The carrier mobility depends on the electric fields generated both by the gate and the drain potentials. Then, the effective carrier mobility μ_{eff} can be expressed by the following equation:

$$\mu_{eff} = \frac{\mu_s}{1 + \mu_s \dfrac{V_{DS}}{v_{\max}\,L}} \quad (2)$$

where μ_s is equal to:

$$\mu_s = \frac{\mu_0}{1+\theta\left(U_{GS}-V_T\right)} \tag{3}$$

Θ is the mobility modulation coefficient which has to be determined in the simulations. v_{max} is the maximal carrier velocity in the channel. μ_0 is the initial carrier mobility. When the transistor is operating in the saturation region, the actual drain voltage V_{DS} must be substituted by the saturation drain voltage V_{DSsat}. The saturation voltage of an ISFET can be expressed as:

$$V_{DSsat} = V_{GS} - V_T + v_{\max}\frac{L_{eff}}{\mu_{eff}} - \sqrt{\left(V_{GS}-V_T\right)^2 + \left(v_{\max}\frac{L_{eff}}{\mu_{eff}}\right)^2} \tag{4}$$

The threshold voltage of an ISFET modified by the surface potential Ψ_s Comparing the above equation to the threshold voltage formula for a simple MOS transistor can be expressed as:

$$V_T^{ISFET} = V_T^{MOS} - \Psi_s - \Phi_m + const \tag{5}$$

where:
V_T^{ISFET}, V_T^{MOS} *– ISFET and MOSFET threshold voltages*
Φ_m *– metal work function*

The constant represents in the equation all the other potential drops independent from the current hydrogen ion concentration. The only one term which is dependent on the chemical composition of the electrolyte is the semiconductor surface potential Ψ_s. The value of the potential for each particular hydrogen ion concentration can be found from the earlier presented chart.

MEASUREMENTS

The measured ISFETs were manufacture at the Institute of Electron Technology in Warsaw, Poland. The transistors possess a built-in channel 640 µm wide and 14 µm long. For technological compatibility reasons, the gate insulator was manufactured as a composite of silicon oxide and nitride.
The measurements were performed on the especially designed measurement stand described in [7]. The stand allows fully automated measurements of several transistor characteristics with various ion concentrations at different temperatures. The presented measurements were taken simultaneously for 10 ISFETs with the hydrogen ion concentration pH equal to 4, 7 and 10.
Unfortunately, only 7 out of the 10 transistors mounted in the measurement unit were working properly. Consequently, all the defective transistors were not taken into account in the simulations. The output and transfer characteristics of the other 7 transistor measured at the pH value equal to 7 are presented in Figures 4-5 respectively. All the measurement points were retained intentionally in the figures so as to visualise the spread in the characteristics between the individual transistors.

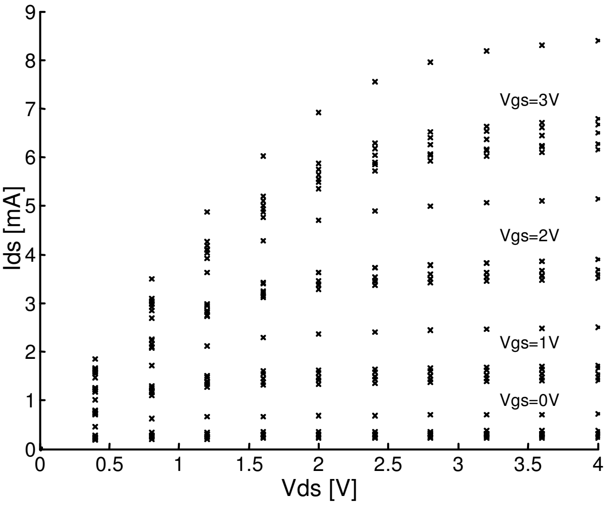

Figure 4: Measured output ISFET characteristics - pH=7

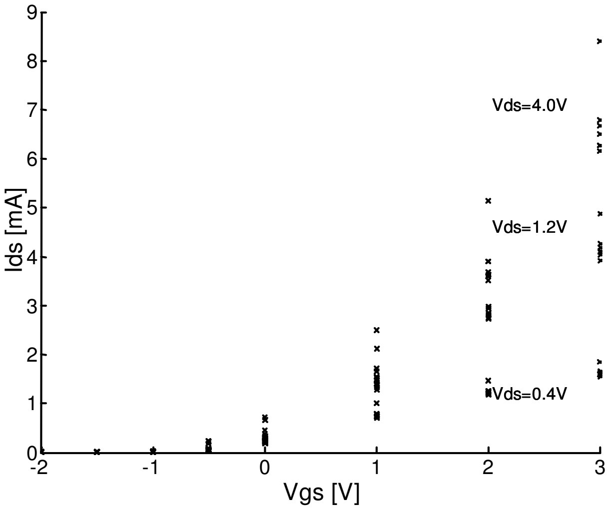

Figure 5: Measured transfer ISFET characteristics - pH=7

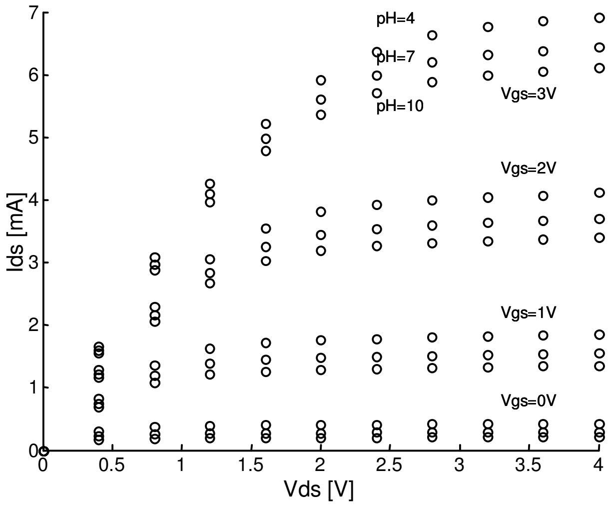

Figure 6: Average measured transfer ISFET characteristics - pH=4, 7 and 10

The above figures allowed the identification of another transistor which differed too much from the others and had significantly higher drain current under the same polarisation. Therefore, this transistors was also not taken into account in the model parameter extraction procedure described in the following section.

Additionally, the measured output characteristics obtained for different pH values averaged for all the sensors, except for the three defective ones and the one having much higher drain current, are presented in Figure 6. As can be seen the ISFET characteristics resemble indeed the ones of an ordinary MOSFET. The threshold voltage estimated from the figures amounts to –0.4 V.

SIMULATIONS

Parameter extraction

The SPICE model parameter extraction was performed based on the presented measurement results. Since the channel dimensions and the electrode voltages were known, the only parameters left to be determined in Equation 1 describing the drain current were the threshold voltage V_T, the surface gate capacitance C_{ox} and the low electrical field carrier mobility μ_0. The capacitance can be calculated directly from the technological data as the series connection of two 50 nm thick capacitors made of silicon oxide and nitride. Thus, only the value of the mobility had to be determined. The capacitance was found to be equal to $4.54 \cdot 10^{-4}$ F/m^2.

Moreover, Equations 2-3 describing the carrier mobility contain two unknown quantities modifying the low electrical field mobility μ_0: the mobility modulation coefficient Θ and the maximal carrier velocity v_{max}. Summarising, there are altogether four ISFET model parameters which are to be determined in the extraction procedure: the threshold voltage V_T, the mobility modulation coefficient Θ, the carrier mobility μ_0 and the maximal velocity v_{max}.

The parameter extraction was performed employing a Newton-Gauss method based automatic procedure already implemented in the Matlab software package. The procedure uses the Least Mean Squares (LMS) optimisation criterion so as to find the optimal set of parameters. For the extraction, all the measurement points were considered, except for the two defective transistors. The extracted optimal, in the LMS sense, values of the model parameters are given in Table 1. The output and transfer characteristics obtained for the optimal parameter values transistor are presented in Figures 7-8 respectively. The solid lines correspond to the fitted characteristics for the improved model. For comparison purposes, the dashed lines represent the fitting results for the original simple SPICE Level 1 model. The circles denote the average measured values for the six properly working transistors.

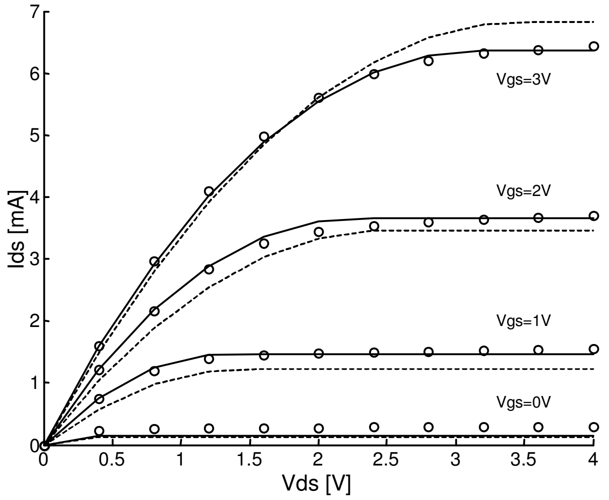

Figure 7: Simulated and measured output characteristics - pH = 7

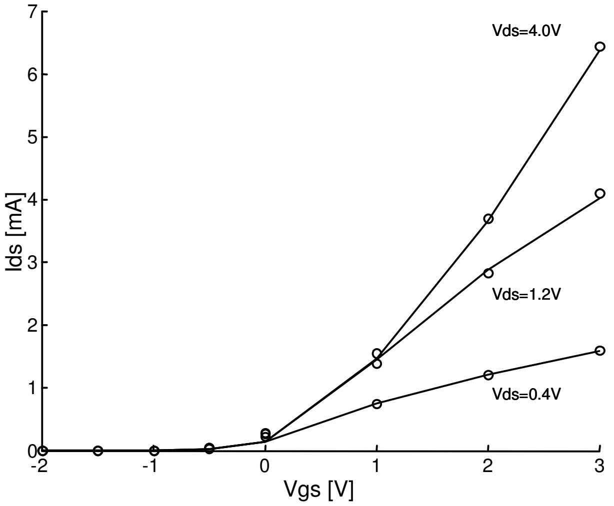

Figure 8: Simulated and measured transfer characteristics - pH = 7

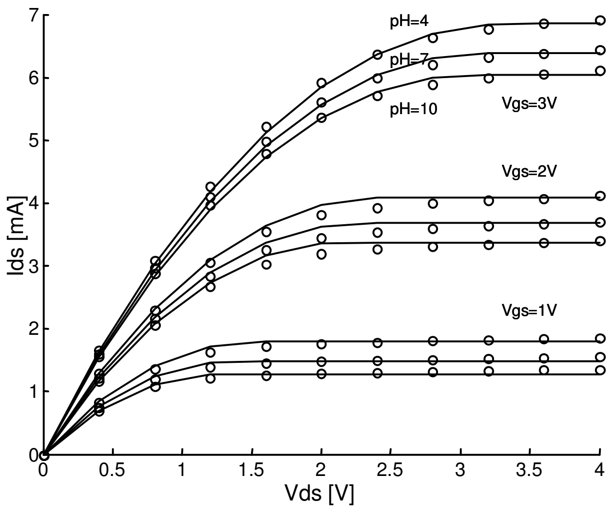

Figure 9: Simulated and measured output characteristics for different pH values

TABLE 1 – Extracted parameters

Parameter	Value	Unit
Threshold voltage V_T	-0.368	[V]
Low field carrier mobility μ_0	0.0970	[m^2/Vs]
Maximal carrier velocity v_{max}	$1.00*10^5$	[m/s]
Mobility modulation coefficient Θ	0.176	[V^{-1}]

As can be seen from the figures, the fitted curves for the improved model match almost perfectly the measured values, whereas such a good fit could not be attained when using the SPICE Level 1 model, which proves that the proposed improvements to the model were justified.

PH sensitivity

The main objective of this part of the simulations was to retrieve the change of the threshold voltage caused by the hydrogen ions present in the gate electrolyte. Thus, this time all the parameters in the simulations, except the threshold voltage, were supposed to have exactly the same values as indicated in Table 1. These values were fitted for the pH value equal to 7. This value of the ion concentration had been expressly chosen so as to minimise the estimation error possibility, because it is close to the so-called Point of Zero Charge (PZC) were the electrolyte induces no charge at the gate insulator surface. Indeed, according to [8] for the silicon nitride used as a gate material this point should be located between the pH values of 7 and 8.

Thus, it was assumed that the only unknown parameter changing with the concentration of the hydrogen ions was the threshold voltage. The corresponding values of the threshold voltage extracted for the hydrogen ion concentration pH equal to 4, 7 and 10 were –528 mV, –368 mV, –245 mV respectively. This yields the gate surface potential shift of 160 mV between the pH values 4 and 7 and 123 mV between the pH values 7 and 10, whereas the expected theoretical value computed from the model should be in both cases equal to 159 mV (see Figure 3).

Thus, the measured sensitivity for the acid solutions matches perfectly the theoretical one and amounts to 53 mV per decade of the ion concentration change. On the other hand, for the basic solutions the sensitivity drops down to only 41 mV per decade. This discrepancy could be explained by the poor quality of the gate dielectric. Then, bearing in mind that the pH values are the logarithmic function of hydrogen ion concentration, for low ion concentrations, the ISFET becomes more vulnerable to the presence of other ions than the hydrogen ones. These so-called disturbing ions bind with the active sites in the gate dielectric instead of the hydrogen ions hence degrading the ISFET sensitivity. This results in the appearance of a bending in the surface potential vs. pH characteristics, i.e. it becomes more flat for high pH values. The detailed consideration on the influence of disturbing ions can be found in [9].

CONCLUSIONS

The main goal of this paper was to present a simple but accurate model of the ISFET. The model is based on a modified SPICE MOS transistor electrical model in which the threshold voltage is influenced by the gate surface potential appearing due to the presence of the hydrogen ions in the electrolyte flowing over the gate.

The model was validated with the measurements of real ISFETs. The model parameters were identified based on the measurements. The simulations performed for the extracted optimal parameter values showed quite good agreement with the measurements.

Moreover, when the electro-chemical model of the phenomena occurring in a particular ion selective membrane is known, the presented model can be easily adapted and applied for the analysis of any other FET–based ion sensor (CHEMFET) as well.

Additionally, the model can be implemented without any difficulties in some Hardware Description Language (VHDL-AMS or Verilog) which allows for behavioural modelling of complex microsystems. The multidomain behavioural modelling has many advantages. First of all, all the analogue and digital components of a system can be simulated in a single environment. Moreover, if required, some thermal, mechanical or chemical sensors might be incorporated in the simulations as well. For example, this approach was already successfully employed by the authors for the multidomain simulation of water pollution monitoring system [9]. There, the smart sensor consisting of an ISFET and an analogue–digital Σ–Δ converter were simulated using the VHDL–AMS language in the hAMSter environment.

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