Temperature Compensation of ISFET Based pH Sensor Using Artificial Neural Networks

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***Abstract*—This paper presents a new Machine Learning based temperature compensation technique for Ion-Sensitive Field-Effect Transistor (ISFET). The circuit models for various electronic devices like MOSFET are available in commercial Technology Computer Aided Design (TCAD) tools such as LT-SPICE but no built-in model exists for ISFET. Considering SiO_2 as the sensing film, an ISFET circuit model was created in LT-SPICE and simulations were carried out to obtain characteristic curves for SiO_2 based ISFET. A Machine Learning (ML) model was trained using the data collected from the simulations performed using the ISFET macromodel in the read-out circuitry. The simulations were performed at various temperatures and the temperature drift behavior of ISFET was fed into the ML model. Constant pH (predicted by the system) curves were obtained when the device is tested for various pH (7 and 10) solutions at different ambient temperatures.**

***Index Terms*—ISFET; SPICE; Machine Learning; Artificial Neural Networks; Macromodel**

I. Introduction

ISFET was first introduced more than 40 years ago in 1972 by Bergveld. Since its invention, ISFET has become a popular platform for chemical as well as biological sensing. Its applications and prospects have become important in the area of biotechnology [1]. ISFETs work on potentiometric technique which has many favorable characteristics, which include high speed, high sensitivity, improved SNR, inherent scalability, low cost, miniaturization and CMOS compatibility [2]. Although conventionally a pH sensor, ISFET has also been used to measure the concentration of ions such as Na^+ or K^+ in a solution [1]. The device characteristics of ISFET are temperature dependent due to thermal agitation affecting the electron flow [3].

Over the past several years, Machine Learning has seen widespread usage and applications to various complex computing problems [4]. With advances in recent research, sophisticated Machine Learning algorithms have been developed which surpass human and hardware performance. Artificial Neural Networks (ANNs) are a prominent class of Machine Learning algorithms [5]. ANNs are a computational model which is based on a large collection of simple, interconnected processing units, which process information by their dynamic state response to external inputs.

This work introduces a novel approach to make the system output of ISFET less sensitive to changes in the temperature. The proposed system consists of ISFET read-out circuit with the temperature compensation incorporated using an ANN model. The neural network is trained using the data obtained from the interfacing circuitry of the device used in different pH solutions at different ambient temperatures. We created an ISFET behavioral macromodel for LT-Spice that can be used for software simulations. The Fig. 1 shows the flow of our work towards temperature compensation, which is explained in detail in Section V.

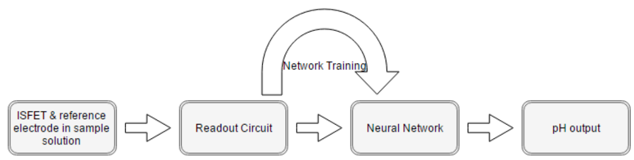

Fig. 1. Design Pipeline

The organization of this paper is as follows: Section II provides an overview of ISFET theory. The SPICE macromodel of ISFET is provided in Section III, while Section IV describes readout circuitry used to carry out the simulations. Section V describes the ANN model used for Machine Learning. Further, the results obtained for temperature compensations are given in Section VI. Finally, we conclude in Section VII.

II. Ion-Sensitive Field-Effect Transistor

ISFET is similar to a MOSFET with a separated gate terminal known as reference electrode. The reference electrode is in contact with the solution and used to supply voltage to modulate the channel current. The gate oxide acts as a sensing film, which interacts with the analyte of interest to produce charges at the electrolyte-insulator interface. The amount of charge generated is a function of the sensing film used and pH of the solution [1]. The electrical schematic of ISFET is demonstrated in Fig. 2.

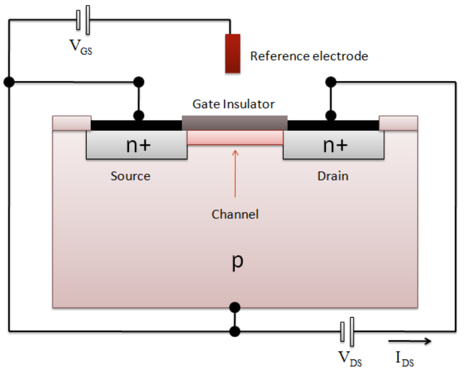

Fig. 2. Schematic diagram of ISFET.

A. The Working Principle

The binding of ions results in accumulation or depletion of carriers in the conducting channel, affecting the threshold voltage of the transistor. This change in V_{th} can be extracted as a change in voltage or current as the output which enables the device to sense the change in ion concentration.

Since the inversion layer is obtained using oxide-electrolyte interface and reference electrode, the threshold voltage expression in ISFET is different from MOSFET [1]. Thus, the effect of reference electrode, the interface between electrolyte and the gate oxide can be seen in the expression of flatband voltage.

$$V_{TH} = E_{ref} - \psi_o + \chi^{sol} - \frac{\phi_{Si}}{q} - \frac{Q_{ss} + Q_{ox} + Q_B}{C_{ox}} + 2\phi_F \quad (1)$$

where, E_{ref}: Reference electrode potential (relative to vacuum); ψ_o : Surface potential resulting from a chemical reaction governed by oxide surface group dissociation; X^{sol}: Surface dipole potential of the solution (a constant); ϕ_{Si}: Substrate (Si) Work Function; q: Elementary charge; $Q_{ss} + Q_{ox} + Q_B$: Accumulated charge at the oxide silicon interface, in the oxide, and the depletion charge in the silicon respectively; C_{ox}: Oxide capacity per unit area; ϕ_F: Fermi Potential.

The expression for ISFET drain current in linear region is similar to that of MOSFET:

$$I_{DS} = K_p[(V_{GS} - V^*_{TH}) - \frac{V_{DS}}{2}]V_{DS} \quad (2)$$

where, I_{DS} = Drain to Source current; K_p = Transconductance parameter; V_{GS} = Gate to Source voltage; V^*_{TH} = ISFET Threshold volatge; V_{DS} = Drain to Source voltage.

The site-binding model explains the mechanism of oxide surface charge creation [6]. It explains the equilibrium between H^+ and OH^- sites on the surface. The charges and capacitances can be described by electrical double-layer theory derived from Gouy-Chapman-Stern model in the electrolyte [7].

B. Temperature Dependence

Mobility (μ) and threshold voltage are the parameters which are significantly affected by temperature (T) change. The dependence on mobility on temperature is

$$\mu(T) = \mu(300K).(\frac{300}{T})^n \quad (3)$$

Dependence of threshold voltage on temperature is reflected in Fermi potential (ϕ_F) variation with temperature (T).

$$\phi_F = \frac{kT}{q} ln \frac{N_{sub}}{n_i} \quad (4)$$

where, N_{sub} is the substrate doping, n_i is the intrinsic carrier concentration (also temperature dependent) and k is Boltzmann constant.

III. LT-Spice Macromodel of ISFET

ISFET is modeled in two stages, viz. the electronic stage, a coupled n-channel MOSFET and an electrochemical stage, which leads to a behavioral macromodel of ISFET [8-9]. The parameters used for the simulation of ISFET were taken from the ISFET fabricated in the Institute laboratory [10-11].

LT-Spice was used to create the sub-circuit model for ISFET (Fig. 3.). It consists of 5 terminals: Drain (D), Bulk (B), Source (S), Reference electrode (ref) and a pH input (pH , modeled as an independent voltage source) which reflects the analyte electrochemical input.

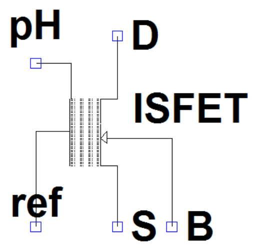

Fig. 3. ISFET LT-Spice Circuit Model

IV. The Read-out Interface Circuit

An interface circuit was created for the ISFET LTspice model developed in the previous section [12-13]. This makes a complete system which is used to detect the ion concentration (H^+ ions). The no load interface circuit for ISFET is demonstrated in Fig. 4., the op-amp $U2$ (in voltage buffer mode) keeps the D terminal at V2 (5V) and op-amp $U3$ keeps the voltage at S constant and hence voltage across resistor, causing the current through ISFET ($U1$) constant, thus, exploiting the feedback and very high gain property of op-amps. The constant I_{DS} and V_{DS} keeps ($V_{GS} - V_{TH}$) constant. Thus, any change in threshold voltage gets reflected to V_{GS} (and hence to V_{Ref}).

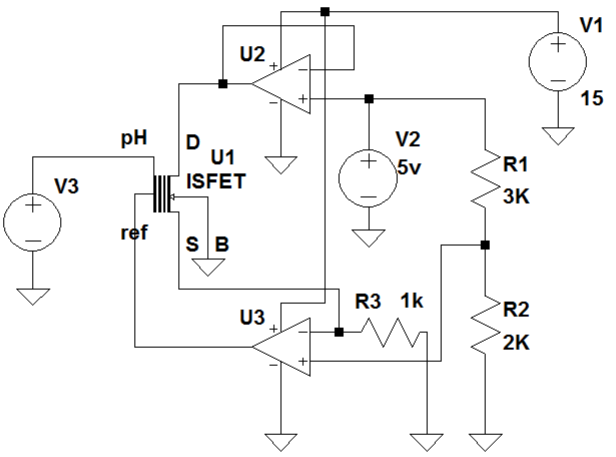

Fig. 4. Complete LT-SPICE Interfacing for ISFET

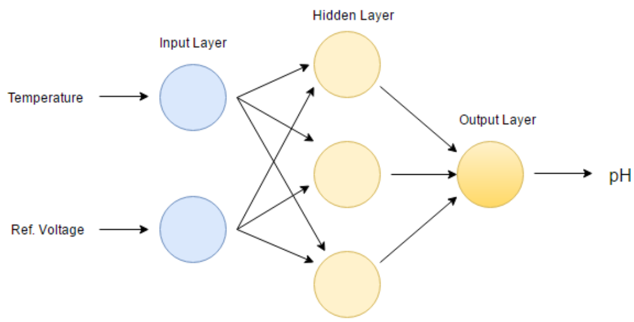

Fig. 5. A 2-input 1-output double layer model

V. Interfacing With Neural Network

A representative two-layer neural network with two input neurons and output neuron is shown in Fig. 5.

A. *Temperature compensation using Neural Networks*

For temperature compensation of the ISFET-based pH sensor, a function is required that relates pH with V_{ref} and temperature. It is difficult to analyze this relation using hardware and therefore a more heuristic approach was adopted to solve the problem.

B. *A Neural Network for SiO_2 based ISFET*

Several dielectrics such as $SiO_2, Si_3N_4, Ta_2O_5, Al_2O_3$ etc. have been used in the past as sensing film [8-9]. In this work, we have analyzed the performance of SiO_2 as the sensing film. The simulation requires a number of surface sites and dissociation constants corresponding to sensing film used in the ISFET, which is introduced in the behavioral model of LT-Spice accordingly [9-10].

1) Data Preprocessing: The preprocessing techniques that we have used are mean centering and normalization, using the variance from the data. Centering and normalization are used for performing 'feature scaling', which is required to obtain the input data on the same scale.

2) The Network Architecture: An optimization strategy was used to optimize the number of neurons in the hidden layer and it was found that 30 neurons in the hidden layer produced the best results. The network is a simple fully-connected feedforward architecture, which has been trained through back-propagation without momentum and weight-decay. The learning rate was decided to be 0.01 through validation.

3) Training Methodology: The simulation was done using $PyBrain$ python library in python3.5 [14]. The dataset was generated using sample points from the pH response of SiO_2-based ISFET device at different temperatures. The reference voltage is plotted against the pH, which was varied from 0 to 13 with a precision of 0.1. Such curves were analyzed for different temperatures $\{15, 20, 25, 30, 35, 40, 45, 50, 55\}°C$. The whole data was split into training, validation and testing datasets in the ratio of 70:15:15. The mean and the standard deviation were calculated on the training data and these values were used to normalize each of the training, validation and testing data. The training was performed upto a maximum of 5000 epochs. The learning rate was fixed at 0.01, while the other hyperparameters were fixed at 0. During validation, the training and testing errors were stored and plotted against the no. of epochs during training. During testing, the trained model was used for prediction. The testing data is used to generate a final testing error. The training error for the SiO_2-based ISFET device was found to be 0.01.

VI. Results and Discussions

A. *Sensitivity Analysis of SiO_2*

Fig. 6. shows the output characteristic curve for SiO_2 sensing film at different temperatures and pH values. The Vref output was observed to be less varying for pH less than 4 while the change is significant for pH more than 4.

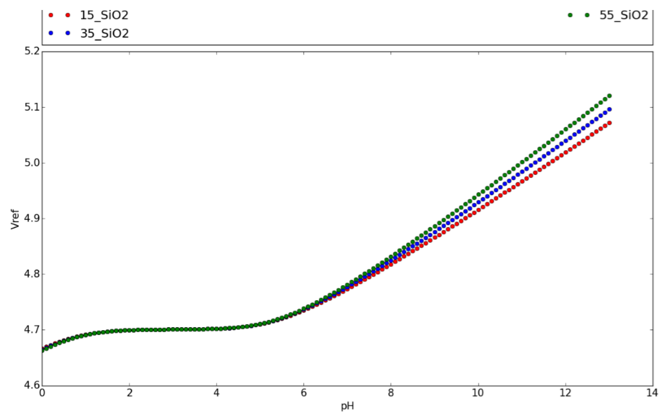

Fig. 6. Vref v/s pH characteristic curve of SiO_2 at different temperatures

B. *Predicted pH v/s temperature curves at pH 4, 7 and 10*

Fig. 7, 8 and 9 shows the predicted pH v/s temperature curve with compensation (Blue) and without compensation (Red)

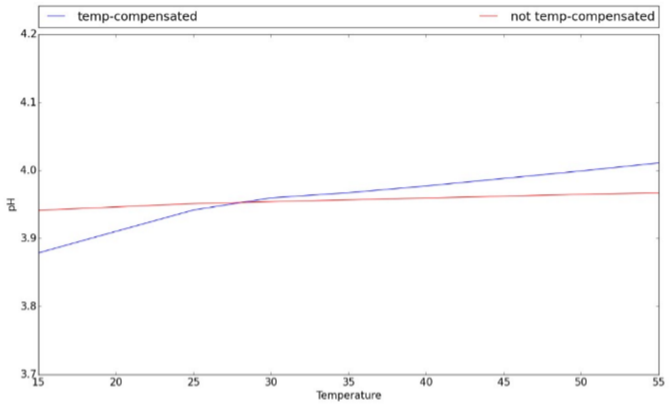

Fig. 7. pH-4 v/s Temperature curve with and without compensation

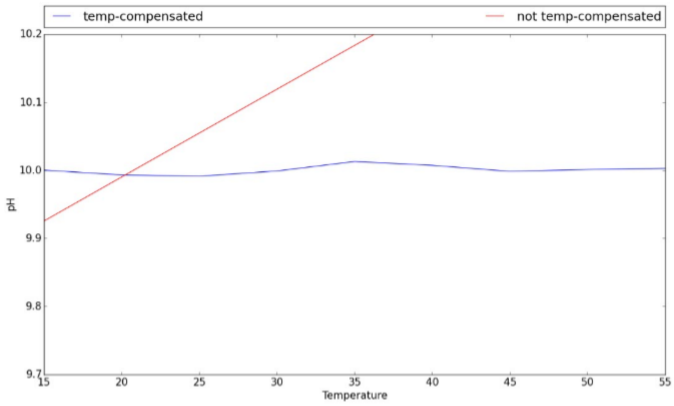

Fig. 9. pH-10 v/s Temperature curve with and without compensation

given the actual pH is 4, 7 and 10 respectively. The blue curve corresponding to pH 4 is varying with temperature instead of being constant. It is because of the less sensitivity of SiO_2 at lower pH values. The desired constant curve was observed with pH 7 and 10 where the system output with compensation (for pH greater than 4) is fairly constant while the response without compensation is varying and significant.

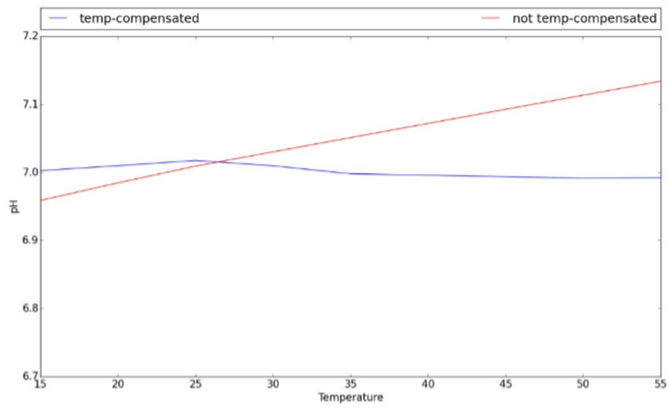

Fig. 8. pH-7 v/s Temperature curve with and without compensation

VII. Conclusion

In this paper, a new technique for ISFET temperature compensation was demonstrated. A behavioral macromodel of ISFET was created in LT-Spice and its characteristic curves were analyzed. The ANN model was trained with the simulation data obtained using the readout circuit and tested with different data points. The desired temperature independent output was observed for pH greater than 4. The Machine Learning Technique, ANN, proved to be quite efficient for temperature compensation.

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