Design and Modelling of Smart Sensor Dedicated for Water Pollution Monitoring

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ABSTRACT

The aim of the paper is to present the smart sensor dedicated for water pollution monitoring. It consists of the ISFET (H^+ ion sensitive field effect transistor) sensor and analogue–digital converter. H^+ sensor can be easily replaced by any other FET–based ion sensor. The need of suitable model creation is stressed. The model of ISFET sensor as well as A/D convereter and their implementation in VHDL–AMS is presented. Finally the results of mixed signal simulation in VHDL–AMS are shown. The analysis of the whole microsystem is performed taking into account the presence of other than hydrogen ions – so called disturbing ions in the measured solution. The analysis of the possibilities of implementation of the best possible kind of the analogue–digital converter was undertaken too.

In the Department of Microelectronics and Computer Science the first approach to the ion identification from the matrix of ISFET/CHEMFET sensors was performed and considered. It uses the neural network for disturbing ion identification and estimation of their concentration.

Keywords: CHEMICAL SENSOR, VHDL–AMS, MICROSYSTEM, CADENCE, MIXED SIGNAL SIMULATION

1 INTRODUCTION

The new standard – VHDL–AMS (Very High Speed Hardware Description Language – Analogue Mixed Signals) was introduced some time ago. The main aim of introducing the new standard is unification of currently existing hardware description languages and (as in case of VHDL) making the technology independent libraries of models that could be accessible by other users or designers.

Setting up a new standard for hardware description language caused, that many VHDL-AMS simulators appeared. As an example the Advance MS by Mentor Graphics can be denoted which soon is going to replace the ELDO ANACAD environment with Hdl–A as an integrated description language. From the non-commercial packages the SOVAMS can be considered [6]. SOVAMS as a new tool is still developed. It consists mainly of the two parts. VHDL–AMS compiler and SPICE OPUS environment.

2 MODEL OF THE ISFET SENSOR IN VHDL–AMS

In this paper the model of ISFET sensor in VHDL-AMS is presented. The modelling of the Ion Selective Field Effect Transistor has been undertaken by many authors [1–4]. The work of the ISFET sensor can be well explained by so called "Site-Binding Theory". It assumes that potential of the solid liquid interface (in this case insulator over the FET's gate – measured solution) depends on the concentration of the hydrogen ions in mentioned solution. The ions from the solution react with the active sites of the insulator either positively or negatively charged. The process of creation of the pairs "hydrogen – active site" changes the total value of the charge of the active sites on the surface of the insulator which influences the transistor's channel current.

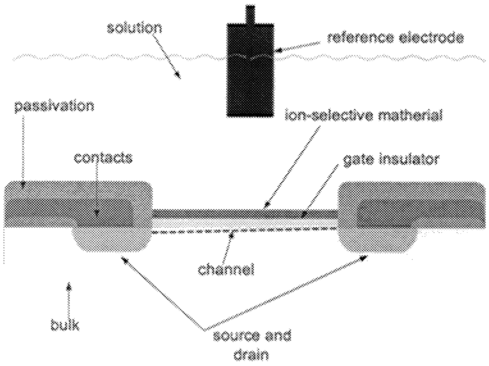

Fig.1 Cross section of ISFET sensor

The most important reaction influencing the transistors current can be written as follows:

$$SiOH_2^+ \xleftrightarrow{kb} SiOH + H_s^+ \tag{1}$$
$$SiOH_2^+ \cdot kb = [SiOH][H_s^+]$$

$$SOH \xleftrightarrow{ka} SO^- + H^+ \tag{2}$$
$$[SiOH]ka = [SiO^-][H_s^+]$$

for the silicon nitride as ion selective layer the second type of the sites (amine sites) has to be also taken into consideration and additional reaction is present on the solid-liquid interface:

$$SiNH_2 + H_s^+ \xleftrightarrow{kn} SiNH_3^+ \tag{3}$$
$$[SiNH_2][H_s^+] = kn \cdot SiNH_3^+$$

Furthermore we assume that the active sites react not only with the hydrogen ions but also with other ions presented in the solution. Let us consider the anions and cations of certain concentration [K] and [A], which reacts with the active sites as follows:

$$SiOH_2^+ + A_{AK}^- \xleftrightarrow{kaip} SiOH_2A \qquad (4)$$
$$[SiOH_2^+][A_{AK}^-]\cdot k_{aip} = SiOH_2A$$

$$SiO^- + K_{AK}^+ \xleftrightarrow{kkip} SiOK \qquad (5)$$
$$[SiO^-][K_{AK}^+]\cdot k_{kip} = SiOK$$

where H_s^+ stands for concentration of the hydrogen ions close to the surface of the isolator. The concentration of hydrogen ions is connected with the concentration of these ions in the bulk of the solution by the following relation

$$[H_b^+] = [H_s^+]\exp(-q\Psi_S / kT) \qquad (6)$$

where Ψ_S represents the potential difference between the bulk of the electrolyte and the surface of the insulator.

A_{AK}^+, K_{AK}^- are the concentrations of the disturbing ions on the common plane which is the part of the Helmholtz (as it is seen on fig.2) layer and connected with the adequate bulk concentrations as follows:

$$[A_b^+] = [A_s^+]\exp(-q\Psi_{AK} / kT) \qquad (7)$$
$$[K_b^-] = [K_s^-]\exp(q\Psi_{AK} / kT) \qquad (8)$$

where Ψ_{AK} is the potential difference between the plane formed by adsorbed anions and cations and the bulk of electrolyte.

According to the Guy-Chapman–Stern theory [2,3] on the border insulator- electrolyte the double layer exists as it is shown below on Fig.2. It consists of the diffuse layer and the Helmholtz layer. In our case the Helmholtz layer consists of the layer of adsorbed hydrogen ion and a common plane of adsorbed anions and cations.

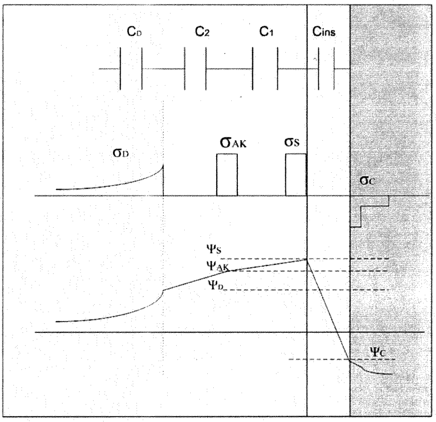

Fig.2 Charge and potential distribution in the solid-liquid interface and electrical representation of the double layer

Assuming that the number of active sites on the surface of the insulator is constant we get the following equations

$$N_{SIL} = SOH_2^+ + SOH + SO^- + SOK + SOH_2A \qquad (9)$$

$$N_{NIT} = SiNH_2 + SiNH_3^+ \qquad (10)$$

The density of the charge on the surface of the insulator can be described as:

$$\sigma_S = e\cdot([SOH_2^+]-[SO^-]+[SiNH_3^+]) \qquad (11)$$

Applying equation 1–5 to 9–11 we can obtain a general dependence of surface charge σ_s to pX where X represents the concentration of certain ion in the measured solution (pX = –log[X])

$$\sigma_S = q\cdot N_{SIL}\cdot\frac{\left(\exp\left(-4.6pH-\Psi_S\frac{q}{kT}\right)-k_ak_b\right)}{\left(\exp\left(-2.3pH-\Psi_S\frac{q}{kT}\right)k_b+\left(1+k_{aip}\left(\exp\left(2.3pA+\Psi_{AK}\frac{q}{kT}\right)\right)\right)\exp\left(-4.6pH-\Psi_S\frac{q}{kT}\right)+k_ak_b+k_{kip}k_ak_b\exp\left(-2.3pK-\Psi_{AK}\frac{q}{kT}\right)\right)} \qquad (12)$$
$$+\,q\cdot N_{NIT}\left(\frac{\exp\left(-2.3pH-\Psi_S\frac{q}{kT}\right)}{\exp\left(-2.3pH-\Psi_S\frac{q}{kT}\right)+k_n}\right)$$

The density of the adsorbed anions and cations on the formed plane can be described as:

$$\sigma_{AK} = e\cdot([K_{AK}^+]-[A_{AK}^-])\cdot N_{AV}\cdot S \qquad (13)$$

where N_{AV} – Avogadro number and S – area of the plane

The charge in the diffuse layer is described in the literature [1,2,4] as follows:

$$\sigma_D = -(8kT\varepsilon_r\varepsilon_0 c)^{\frac{1}{2}}\sinh\left(\frac{ze\Psi_D}{2kT}\right) \qquad (14)$$

To describe the channel surface charge density σ_c the equation introduced by Kingston [13] was applied

$$\sigma_C = \frac{2\varepsilon_0\varepsilon_S kT}{q\sqrt{\frac{2kT\varepsilon_0\varepsilon_S}{p_0q^2}}}\left[\left(\exp\left(\frac{-q\Psi_S}{kT}\right)+\frac{-q\Psi_S}{kT}+1\right)+\frac{n_0}{p_0}\left(\exp\left(\frac{q\Psi_S}{kT}\right)-\frac{q\Psi_S}{kT}-1\right)\right]^{\frac{1}{2}} \qquad (15)$$

The charge neutrality of the system is accomplished by the following equation:

$$\sigma_S + \sigma_C + \sigma_{AK} + \sigma_D = 0 \qquad (16)$$

and charges are related to the potentials by following equations

$$\Psi_S - \Psi_{AK} = -\frac{\sigma_{AK}}{C1} \qquad (17)$$

$$\Psi_{AK} - \Psi_D = -\frac{\sigma_D}{C2} \qquad (18)$$

$$\Psi_C - \Psi_S = \frac{\sigma_C}{C_{ins}} \qquad (19)$$

Above equation form the system which allows to calculate the surface potential vs. concentration of hydrogen ions as well as of concentration of disturbing ions.

In VHDL–AMS we set up all the charges as well as potential as **quantities** the pH, pA, pK values are **input**

terminals whereas the surface potential Ψ_s are **ouput terminal** [5]. It influences threshold voltage of the transistor (transducter) as follows:

$$V_T^{ISFET} = V_T^{MOS} - \Psi_s + const \qquad (20)$$

where: V_T^{MOS} , V_T^{ISFET} represents threshold voltages of the MOS structure and ISFET structure respectively. Constant represents all the other potential drops independent on the current ion concentration.

The complete model of the sensor in VHDL –AMS can be represented as below:

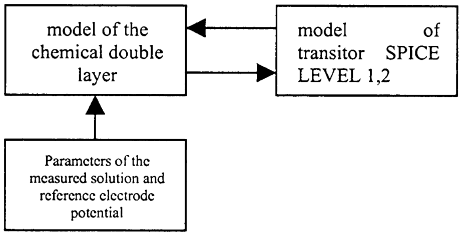

Fig.3 Schematic representation of the model

3 SIMULATION RESULTS

In this section the examplanary curves of the sensor are showed. As it can be seen on Fig. 4 the lower and upper regions of the Ψ_s(pH) curve are influenced by the additional disturbing ions added to the measured solution

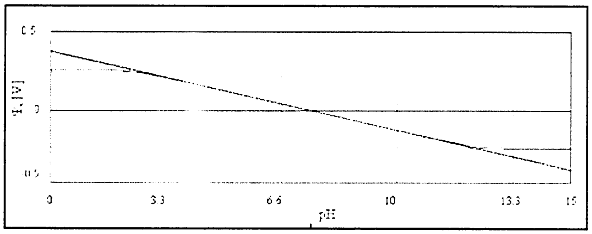

Fig.4 Curve Ψ_s vs. pH with different values of pK and pA for pK=pA=1 the nonlinearities can be seen

Fig.5 and 6 shows the influences of the contents of measured solution on the output curves.

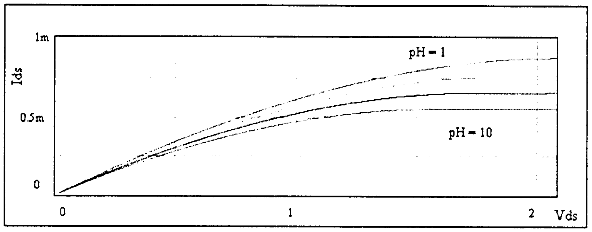

Fig.5 Output curves of the ISFET sensor with V_{gs}=2V and different values of pH = 1,4, 7,10

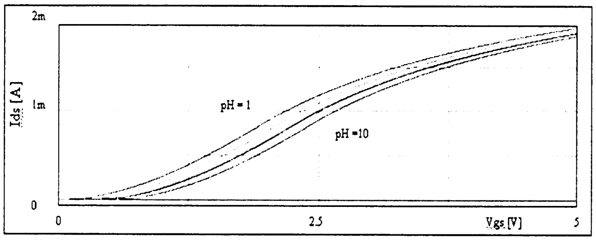

Fig.6 Transfer curves of the ISFET sensor with V_{ds} =1V and various pH=1,4,7,10

4 MODELLING OF THE SIGMA-DELTA ANALOG TO DIGITAL CONVERTER

The second part of the presented microsystem is the data processing unit. It consists of the sigma-delta analogue to digital converter. This circuit belongs to the group of oversampling converters, which exchange resolution in amplitude for resolution in time. Thanks to it the user can match the resolution of the converter depending on required accuracy. This converter can be divided into two main parts: analog and digital. Analogue part consists of sigma-delta modulator and digital part consists of the decimation filter.

5 VHDL-AMS MODEL OF THE SIGMA-DELTA MODULATOR

There are many various architectures of the sigma-delta modulators [7,8,10,11,12]. In this article the 1st order up to 3rd order sigma-delta modulator are presented. The block diagram of the 3rd order sigma-delta converter is shown in figure 7.

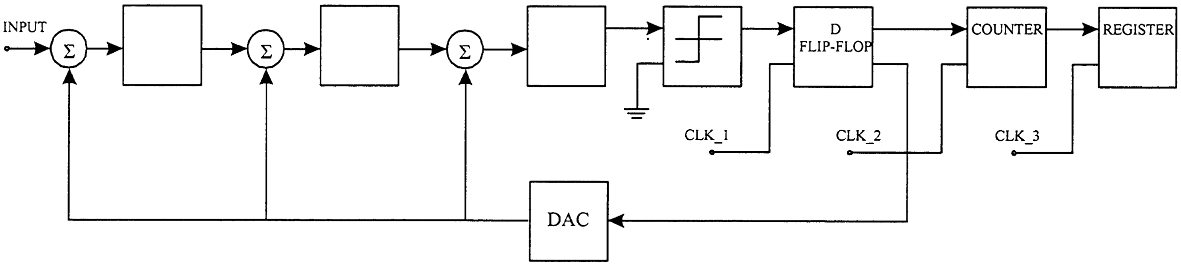

Fig. 7: Block diagram of the data processing unit

As it can be seen the three integrator blocks are placed in the main path of the modulator. The number of the integrator blocks is responsible for the order of the modulator. The increase of the order modulator cause the increase of the signal to noise ratio (SNR) but reveals some problems with stability of the whole modulator. To eliminate this effect the cascade structures of the modulator are used. Authors of this article present the simulation results of the 1st to up to 3rd order sigma-delta converter. However the cascade structures of the modulator are now constantly investigated.

The whole presented modulators are modelled in VHDL-AMS language. It consists of the separate blocks of integrator, comparator, D flip-flop, digital to analog converter and sumation node. All of the blocks are connected using structural description.

6 VHDL-AMS MODEL OF THE DECIMATION FILTER

The second part of the presented analog to digital converter is the decimation filter [7,8,9,10]. On the input of this circuit is a 1-bit binary stream of ones and zeros represents the amplitude of the input signal. This stream is then converted into n-bit binary words using a digital decimation filter. The simplest implementation of this unit uses an 8-bit counter as an averaging filter to return the average value of the sigma-delta modulator output over a fixed period. The 8-bit counter counts at the oversampling frequency and is reset at the end of the OSR cycles where:

$$OSR = \frac{f_s}{f_n} \qquad (21)$$

OSR – oversampling ratio

f_s – oversampling frequency

f_n – Nyquist frequency

The mentioned counter produces an 8-bit binary word. This word is loaded into the output register, which forms the output of the analog to digital converter. The main disadvantage of this solution is that an increase of the analog to digital converter's resolution requires an increase the oversampling frequency.

This part of the converters can be easily modelled using VHDL-AMS because consists only of two blocks: 8-bit counter and 8-bit register. Both units create the decimation filter structures, which can be connected with sigma-delta modulator.

7 ADCONVERTER SIMULATION RESULTS

The whole presented microsystem was fully simulated using VHDL-AMS model of presented structures. To test the behavior of the sigma-delta analogue to digital converter the sinus signal on the input was given. The simulation results of the 1st order up to 3rd order structures of the modulator are shown in figure 8.

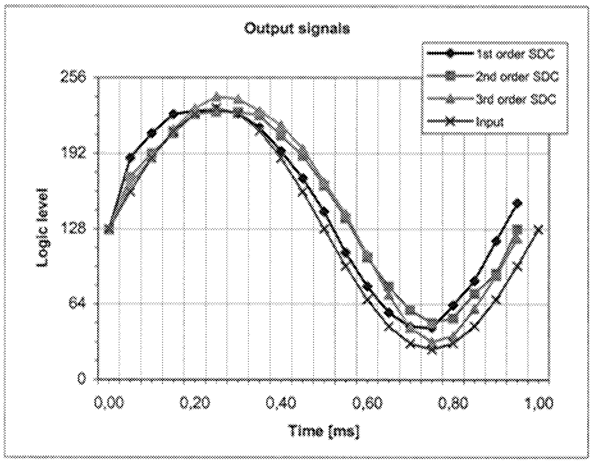

Fig. 8: Simulation results of the analog to digital converter

As it can be observed there are differences between 1st, 2nd and 3rd order sigma-delta converter. The 1st order sigma-delta converter the poorest fitted to the input signal. This corresponds with only one integrator that is used to build sigma-delta modulator. The 2nd order of the modulator fits better whereas the 3rd fits the best. This is connected with noise shaping of the converter that is the best in 3rd order of the converter. Unfortunately in the 3rd order of the modulator there are the greatest problems with stability. That is why the input signal has to be limited.

8 GLOBAL SIMULATION RESULTS

The final step after simulating the sensor part of the system and processing part was the mixed signal simulation of both parts togeter. The sensor was set up in the standard constant current mode circuit that can be found in some papers [4]. The output signal of that circuit that equals:

$$U_{out} = -\Psi_s \qquad (22)$$

was set as an input signal of the converter. After then the global simulation was performed. The results of simulation can be seen of Fig. 9. The nonlinearities in output signal are mainly caused by the nonlinearity of processing part of the system

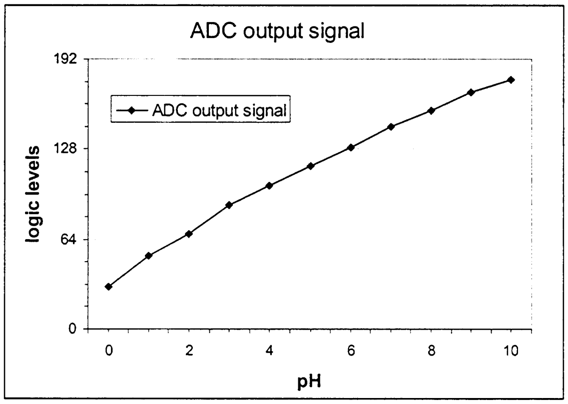

Fig.9 The results of mixed simulation of the sensor and ADC.

Resolution of the converter can be estimated by dividing the maximum range of input signal (1V) by the maximal number of logic levels (for 8 bit it is 256). This gives 3.9mV.

9 CONCLUSIONS

The presented silicon microsystem was fully designed and tested with application of VHDL-AMS language. The obtained results are compatible with authors expectation. The main advantage of using VHDL-AMS standard to describe microsystem model is the cut down the time of the simulation by comparison with model using transistor level. It allows also to perform global mixed signal analysis of the system that is not possible for standard VHDL simulators. Authors of the article are constantly investigated new structures of the microsystem (sensor and also a analog to digital converter architectures) to find the best solution that can be used to water pollution monitoring system. The best solution will be designed using CADENCE environment and implemented in silicon structures.

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