



INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

Stability Analysis of Metal Oxide Gas Sensors Using System Identification

Nimisha Dutta

Electronics and Communication Engineering, PhD, Tezpur University, India

nimisha.dutta0@gmail.com

Abstract

Metal Oxide semiconductor (MOS) gas sensors are thought to be the best to meet the present day technical and economical requirements. The poor selectivity of MOS sensors is improved by the consideration of temperature variation. In this paper, we have made the system identification and stability analysis of MOS gas sensors. Pulse modulation being a popular method of feature extraction of MOS sensors, optimization of parameters of pulse modulation becomes very significant. The selection of the sensor model that provides the most stable and desired sensor response is provided by the system identification technique. Hence the problem of choosing the best frequency and duty cycle of the temperature modulating signal of the MOS sensor is solved. The estimation of model parameters is done using iterative prediction-error minimization (PEM) method. Based on the sensor stability best suited transfer function was chosen for the MOS gas sensors, and then the sensors were operated at the respective best frequencies and duty cycles.

Keywords: Metal Oxide Semiconductor (MOS) gas sensors; Temperature Modulation; System Identification.

Introduction

Metal oxide semiconductor (MOS) based gas sensors have been widely used in gas detection. Their advantages include low cost and high sensitivity along with disadvantages such as lack of stability and selectivity [1, 2]. Practically, several attempts have been made to overcome such drawbacks by using chromatographic columns to separate components, by operating at different temperatures [3]-[6], by choosing different burning-in procedures, dopants, surface chemical modification [7]-[9] etc. By changing the operating temperature of the MOS sensors the response to a given chemical species alters. Many authors have

indicated that modulation of the sensor temperature [10]-[13] provides more information from a single sensor than in isothermal operation, allowing improved research works in gas detection. The modulation of temperature changes the kinetics of the adsorption processes that take place at the sensor surface while detecting reducing or oxidizing species in the presence of atmospheric oxygen leading to the development of response patterns, which are the characteristic of the species being detected. It is desirable to operate the sensors at slow temperature cycles as it increases the duration

of sampling times and hence allows the sensor to reach the stand point temperature which preserves the dynamic characteristics of the sensor.

Previous research work of different groups have shown that the performance of almost all types of SnO₂ sensors is sensitive to the temperature of operation [14,15]. The nonlinear dynamic response of a gas sensor changes characteristically depending on the concentration and chemical structure of gas molecules. Temperature variation approach, which compares and combines the results at different temperatures, is employed for the analysis and exploitation of the information from gas sensors by many of the researchers [14]-[16]. The main characteristic of these methods is the temperature modulation or dynamic measurement technique and thereby to improve the selectivity of the sensors. Many works have been carried on the advantage of temperature modulation on a ceramic metal oxide sensor at two different temperatures to detect the presence of carbon mono-oxide [17]-[19]. Researchers have also reported the temperature modulation using square wave to quantify hydrogen sulphide [20]-[21]. The discrimination between different gases, modulating patterns such as sawtooth, triangular and square was also applied to the sensors [22]. The sinusoidal variation in the temperature also enhanced the classification of different gases. A number of works on the cyclic

variations of the sensor heater voltage have been reported by many authors [23] and [24]. Although the results reached by such works are very promising, the selection of modulation frequencies used in all the previous works are based on trial and error procedure and there is no way to ensure that the frequencies used are optimal for each application or not.

The identification of the mathematical baseline model of the sensor can help simulating the sensor dynamics for different arbitrary temperature functions and frequencies. The selection of the best function and the best frequency to achieve a stable dynamics that follow the concentration of the analyte will be an important optimization strategy of the gas sensor. The instability in the sensor dynamics of the baseline response is also transferred to the sensor response with odour stimulation. System identification through multilevel pseudorandom sequences and pseudorandom binary sequences [25], [26] has been done by researchers that enabled the selection of optimized modulation frequency. Temperature modulation being a popular method of feature extraction of MOS sensors, optimization of parameters of pulse modulation will be a remarkable strategy in this area. The analysis focuses on the system identification of MOS gas sensors that helps to overcome the problem of choosing the best frequency of the temperature modulating signal of the MOS sensor. In this work we have chosen a set of optimized frequencies for the first time in MOS sensors using system identification theory for sensor modeling and hence to find the most stable transfer function.

System Identification Theory and Sensor Model Estimation

System Identification

The phenomenon of system identification is the art of building mathematical models of dynamical systems using experimental data. It is an iterative procedure. The sensor model may be developed either from the physical model or from input output data. Since physical model is difficult to be derived we have used system identification technique. The measurement of the data can be done either in time domain or frequency domain and have single or multiple input-output. The dynamic characteristics of time domain signals include rise time, response rate and overshoot rate. The inputs for time domain analysis is the impulse, step or ramp signals. System identification supports a wide range of linear and nonlinear models, including linear nonparametric models that estimate the impulse and frequency response at each time or

frequency value, linear polynomial and state-space models, and nonlinear ARX structures.

The physical phenomenon of the sensor implies that the MOS sensor models rely on the mechanism of adsorption of gas molecules by the sensor film, under temperature modulation and then the change in the electrical conductance of the sensor material. Although, the above stages looks distinct, physically it is difficult to distinctly segregate the whole model into such distinct stages. This work focuses on the achievement of optimized temperature modulation based on the system identification technique and the best transfer function based on the sensor stability was obtained for the MOS gas sensors.

Model Estimation

To find a model to relate input and output data sequences in the presence of measurement errors and with lack of knowledge about the physical phenomena that relate these data is a highly non-unique, nontrivial problem. To overcome this problem, specific models, model sets, and parameterizations are introduced. System identification computation enables the estimation of linear and nonlinear mathematical models to fit input and output data from dynamic systems. A model of a system describes the system completely and helps simulation of the output of a system for a given input and analyzes the system's response. System identification is applicable to a wide range of linear and non-linear models, including linear non-parametric models that estimate the impulse and frequency response at each time or frequency value, linear polynomial and state-space models and nonlinear ARX structures. The nonlinear system identification of dynamical systems involves structure selection, input sequence design, noise modeling, parameter estimation and model validation.

The Linear Time Invariant (LTI) model in our case implements the continuous time, discrete time, state space, transfer function and zero-pole gain model conversions. The model estimation of is done using iterative prediction-error minimization (PEM) method. This prediction error is the difference between the output of the system as would be predicted by the model and the actual measurement.

State-space models

In the state space form, the relations between the input, noise and output signals is represented as a system of first-order differential equation using an auxiliary state vector $x(t)$. In continuous time, the modeling normally leads to a representation such as-

$$\dot{x}(t) = Fx(t) + Gu(t) \tag{1}$$

where F and G are the matrices of proper dimensions. Since the system identification has been performed from the discrete data of input-output, the discrete state space model is more relevant than continuous time model. The discrete state-space model is given by:

$$x(KT + T) = Fx(KT) + Gu(KT) \tag{2}$$

where K is the sampling instant and T is the sampling interval.

Transfer function stability=

The transfer function of an LTI system is defined as the ratio of the Laplace transform of the output (response function) to the Laplace transform of the input (driving function), provided all the initial conditions are zero. Let $\eta(t)$ be the measurements that would lead to ideal, noise-free sensors given by-

$$\eta(t) = Hu(t) \tag{3}$$

where the transfer function H in Laplace domain can be represented using state-matrices as-

$$\hat{H}(s) = H(sI - F)^{-1} + G \tag{4}$$

and it can be reduced to a form,

$$\hat{H}(s) = \frac{b_0s^m + b_1s^{m-1} + \dots + b_m}{s^n + a_1s^{n-1} + \dots + a_n} \tag{5}$$

Further the z-transform of the LTI model can be represented as-

$$\hat{H}(z) = \frac{b_0z^m + b_1z^{m-1} + \dots + b_m}{z^n + a_1z^{n-1} + \dots + a_n} \tag{6}$$

When the sensor temperature is modulated, the complicated response transients are considered to be related to different reaction kinetics of the gas molecules. At low temperatures mainly surface reactions occur while at high temperatures bulk reactions between point defects in the semiconductor lattice and gaseous oxygen molecules occur. In both cases, the adsorption at active sites occurs first followed by some catalytic reactions. The oxygen adsorbates are partly consumed by oxidation of target gases on the semiconductor surface during the static measurement. The amount of chemisorbed oxygen decreases and hence the conductance increases,

hence, changing the resistance change of MOS sensors which shows that the concentration of chemisorbed oxygen changes at the grain boundary. In the adsorption process the conductance increases with decrease in the concentration of chemisorbed oxygen.

The dynamics of the sensor is greatly influenced by the frequency and duty cycle of the pulse temperature signal. This is because of the fact that the time for the reaction kinetics should match to the time for the sensor heating process. Fig 1 (a) and 1 (b) shows two distinct patterns of sensor responses where in (a) the sensor behaves as in transient mode with an overshoot before coming to a stable and equilibrium response level of 0.02 volt, whereas in (b) the sensor response is fairly stable. In this work we have derived eight different sensor model equations for the pulse frequencies of 10mHz, 40mHz, 80mHz and 120mHz at duty cycles of 50% and 75% in each case. The stability of the models has been verified by calculating the overshoot percentage and from the pole-zero plots. This analysis shows that the sensor models can be chosen with the best dynamic performance based on stability analysis hence determining the corresponding best frequency and duty cycle. The work focuses on the derivation of various transfer functions under stable and unstable modes by PEM technique in MATLAB.

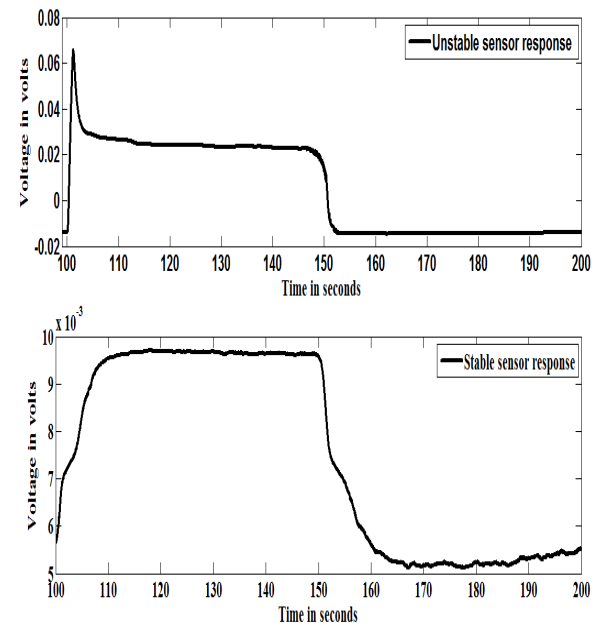


Fig 1. Sensor response on pulse temperature modulation (a) Unstable response for TGS-822 with overshoot (b) Stable response for TGS-2611.

Experimental

Measurement and set-up

The experiment was performed on two MOS gas sensors (TGS-822 and TGS-2611). The dynamic analysis was conducted for different pulse modulating temperature without applying any gas to analyze the baseline response and stability of the sensors. The heater voltage modulation patterns (frequency and duty cycle) of the sensors were controlled by a PC through a Data Acquisition card (PCI6024E, National Instruments) and LabVIEW. The analog output of the card was applied to the gate of a MOSFET which supplies the modulating voltage to the sensors. Therefore, the heater voltage $+V_H$ accordingly followed the pulse signal to excite the sensor. The baseline sensor response was interfaced to the PC through the DAQ card. Two diaphragm pumps controlled by the PC through a driver circuit consisting of relays and transistor switches was used to direct clean air into the sensor head block through teflon pipes. The 'purging' and 'refreshing' sequence was controlled with proper time duration through the DAQ card by the PC using LabVIEW programming. The sensors were kept inside a chamber away from interfering gas so that the baseline is established with clean air. Before each run of data acquisition, the baseline was verified and when found deviated, it was corrected by purging in clean air ensuring that the sensor baseline settles to a fixed level without any interfering gas.

At first, the sensor temperature was pulsed at different frequencies of 10mHz, 40mHz, 80mHz and 120mHz and duty cycles of 50% and 75% duty cycles to generate the sensor responses. The frequency was selected based in a trial and error procedure. The sensor signals were acquired at a sampling frequency of 1 kHz. The stability analysis was performed based on the system identification technique and the frequency and duty cycle was determined for which the transfer function was most stable.

Results and Discussions

The output response for square input pulse for sensor TGS-822 at four different temperature pulse frequencies is shown in Fig. 2. The input-output signal data obtained from the sensor response are then quantified by the system identification process. The model estimation is done by the system identification technique and the stable transfer function is determined based on the pole zero plot and the overshoot percentage. By applying the respective best frequencies and duty cycles to the sensors the classification of different samples were

done and the classification percentage before and after the optimal frequency modulation was found.

Transfer function determination

The transfer function is determined from the input pulse voltage and the output response. To ensure the accuracy of the estimated transfer function, a comparison is made between the simulated and the measured sensor output response. The model is selected on the basis of PEM method. The comparison between the simulated and the measured results of are done. The system identification gives us a transfer function of the sensor model in z-domain with a higher order approximation, however the model can be reduced to a lower order approximation say to order 2 or 1. Based on the pole-zero plots and the overshoot percentage, the best transfer function is selected. Fig.3 shows the pole-zero diagrams of the transfer function and Fig.4 with zoomed visualization. As can be seen all the poles lie strictly inside the unit circle. The distance of the poles from the unit circle is calculated from the transfer function and is tabulated in Table 1.

Another criterion for choosing the stable transfer function is the overshoot percentage calculated from the step response (Fig. 5) of the three sensors. As shown in the table, the optimal frequency and duty cycle obtained for the two sensors were 2mHz and 50% duty cycle and 1mHz and 50% duty cycle respectively. It can also be seen that as the frequency increases, the stability decreases. Hence, the sensors are more stable at lower frequencies.

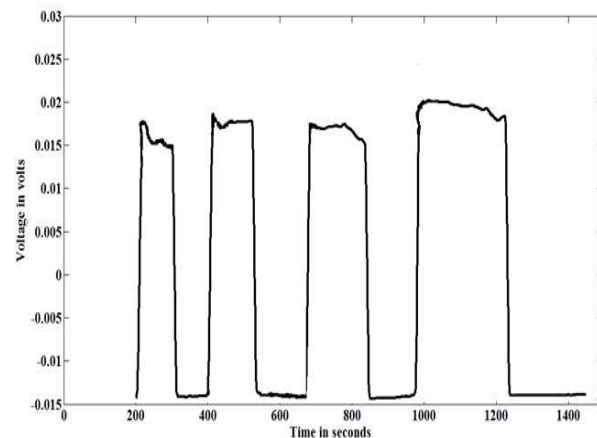


Fig. 2 Sensor response at four different frequencies of 2mHz, 3mHz, 4mHz and 5mHz

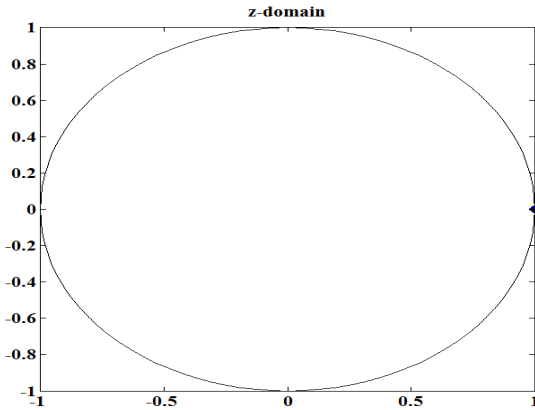


Fig. 3(a). Pole-zero plot of transfer function of sensor TGS-2611 in z-domain at 2mHz and 50% duty cycle.

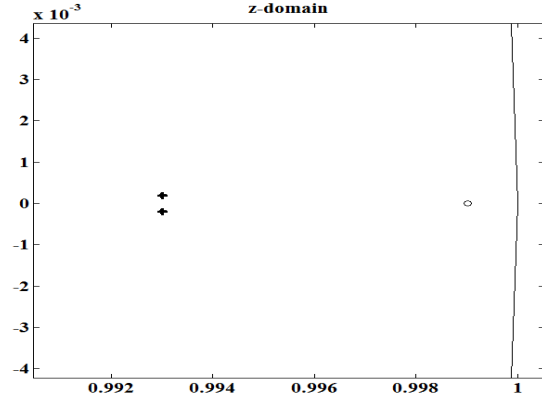


Fig. 4(b). Zoomed part of the pole-zero plot of transfer function of sensor TGS-822 in z-domain at 1mHz and 50% duty cycle.

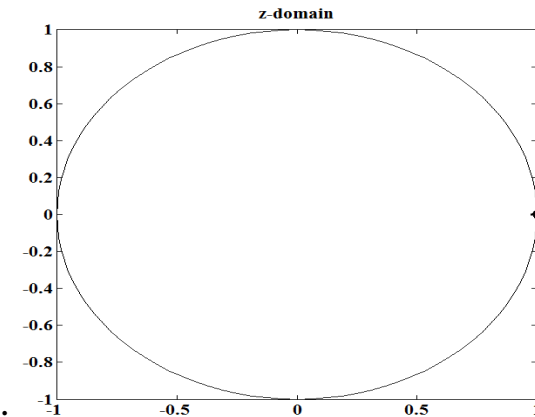


Fig. 3(b). Pole-zero plot of transfer function of sensor TGS-822 in z-domain at 1mHz and 50% duty cycle.

Table 1. Transfer function model parameters of the MOS sensors for different frequencies and duty cycles (The stable model parameters are shown in bold):

Sensors	Frequency (mHz)	Duty Cycle (%)	Percentage of overshoot (%)	Position of pole from centre	Stability	Stable Transfer Function
TGS-2611	1	50	0.08	0.996,0.9982	Unstable	$\hat{H}(z)_{\text{stable}} = \frac{(5.902 \times 10^{-7})(z - 0.9989)}{(z - 0.995)(z - 0.996)}$
	2		0.004	0.995,0.996	Stable	
	3		1.02	0.998,0.9997	Unstable	
	4		1.09	0.9996,0.9999	Unstable	
	5		2.15	1.0008,0.9998	Unstable	
	10	3.27	1.0005,1.0003	Unstable		
	1	75	1.6	0.999,0.9998	Unstable	
	2		1.7	0.9998,0.9999	Unstable	
	3		2.23	0.999,1.0003	Unstable	
	4		3.41	0.9998,0.9999	Unstable	
5	3.37		1.0002,1.0005	Unstable		
10	4.52	1.0006,0.9999	Unstable			
TGS-822	1	50	0.09	0.992,0.9938	Stable	$\hat{H}(z)_{\text{stable}} = \frac{(2.791 \times 10^{-7})(z - 1.00035)}{(z - 0.992)(z - 0.9938)}$
	2		1.087	0.9993,0.9997	Unstable	
	3		1.285	0.999,0.9999	Unstable	
	4		3.97	1.0.9999	Unstable	
	5		4.28	1.0003,1.0005	Unstable	
	10	5.64	1.0008,1.0009	Unstable		
	1	75	1.15	0.9996,0.9999	Unstable	
	2		1.96	0.996,0.9998	Unstable	
	3		2.156	0.999,1.0002	Unstable	
	4		3.37	0.999,1.0004	Unstable	
5	3.88		1.0005,1.0009	Unstable		
10	4.16	1.0006,0.9999	Unstable			

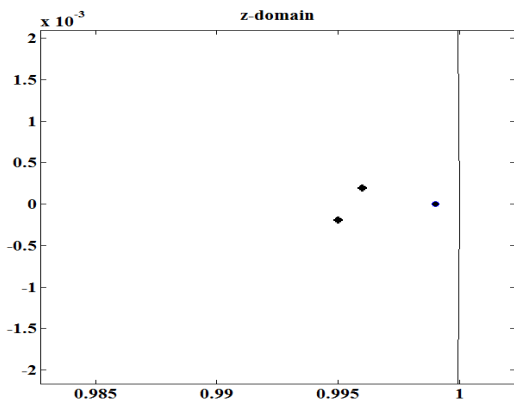


Fig. 4(a). Zoomed part of the pole-zero plot of transfer function of sensor TGS-2611 in z-domain at 2mHz and 50% duty cycle

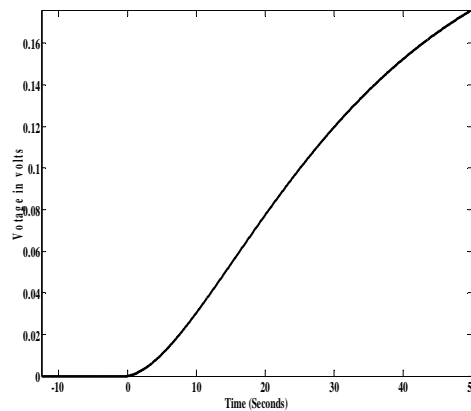


Fig. 5(a). Step response of sensor TGS-2611 at 1mHz and 50% duty cycle.

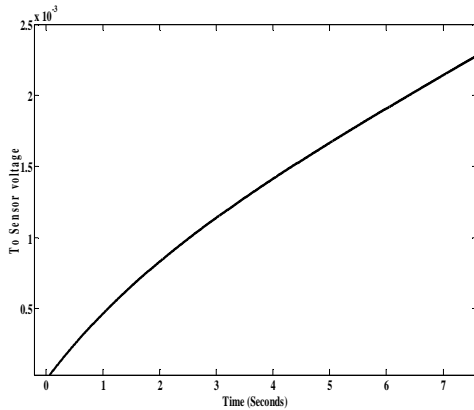


Fig. 5(b). Step response of sensor TGS-822 at 2mHz and 50% duty cycle.

Conclusions

In this paper a study aimed at the selection of optimized frequencies and duty cycles based on system identification technique is presented. The method is applied to study the stability of MOS based gas sensors and the transfer function determination based on the pole-zero plot and the overshoot percentage. The frequencies and duty cycles at which the transfer function was most stable for TGS-2611 and TGS-822 was determined as 2mHz and 50% and 1mHz and 50% respectively.

It is seen that the system identification technique could effectively find the modulation frequencies at which the system is most stable which could be further applied for gas analysis applications.

References

- [1] K.Ihokura, J.Watson, *Stannic Oxide Gas Sensors, Principles and Applications*, CRC press, Boca Raton, FL,1994.
- [2] P.Mosely, B.Tofield, *Solid state gas sensors*, Adam Hilger, Bristol 1987.
- [3] Andrew P. Lee, and Brian J. Reedy, *Temperature modulation in semiconductor gas sensing*, *Sensors and Actuators B* 60 (1999), 35-42.
- [4] A.Heiling, N. Barsan, U. Weimar, M. Schweizer-Berberich, J.W. Gardner, W. Göpel, *Gas Identification by Modulating Temperatures of SnO₂-Based Thick Film Sensors*, *Sensors and Actuators B* 43 (1997), pp-45-51.
- [5] Xingjiu Huang, Fanli Meng, Zongxin Pi, Weihong Xu, and Jinhuai Liu, *Gas sensing behavior of a single tin dioxide sensor under dynamic temperature modulation*, *Sensors and Actuators B* 99 (2004) 444–450.
- [6] A. Vergara, E. Llobet, J. Brezmes, X. Vilanova, M. Stankova, I. Gracia, C. Cane,

- X. Correig, “Optimized multi-frequency temperature modulation of micro-hotplate gas sensors”, *IEEE Sensors Journal*, 2004.
- [7] N. Barsan, R. Ionescu, A. Vancu, *Calibration curve for SnO₂-based gas sensors*, *Sens. Actuators B* 18–19 (1994) 466–469.
- [8] U. Weimar, W. Göpel, *AC measurements on tin oxide sensors to improve selectivities*, *Sens. Actuators B* 26 (1995) 13.
- [9] K. Wada, M. Egashira, *Improvement of gas-sensing properties of SnO₂ by surface chemical modification with diethoxydimethylsilane*, *Sens. Actuators B* 53 (1998) 147–154.
- [10] Andrew P. Lee, and Brian J. Reedy, “Temperature modulation in semiconductor gas sensing”, *Sensors and Actuators B* 60 pp. 35-42. (1999).
- [11] A.Heiling, N. Barsan, U. Weimar, M. Schweizer-Berberich, J.W. Gardner, W. Göpel, “Gas Identification by Modulating Temperatures of SnO₂-Based Thick Film Sensors”, *Sensors and Actuators B* 43 ,pp-45-51,1997.
- [12] Xingjiu Huang, Fanli Meng, Zongxin Pi, Weihong Xu, and Jinhuai Liu, “Gas sensing behaviour of a single tin dioxide sensor under dynamic temperature modulation”, *Sensors and Actuators B* 99 ,pp. 444–450, 2004
- [13] A. Vergara, E. Llobet, J. Brezmes, X. Vilanova, M. Stankova, I. Gràcia, C. Cané, X. Correig, “Optimized multi-frequency temperature modulation of micro-hotplate gas sensors”, *IEEE Sensors Journal*, 2004.
- [14] A. Heilig, N. Barsan, U. Weimar, M. Schweizer- Berberich, J.W. Gardner, W. Göpel. *Gas identification by modulating temperatures of SnO₂ based thick film sensors*, *Sensors and Actuators B*, Vol. 43, 1997.
- [15] A.Ortega, S. Marco, A. Perera, T. Sundic, A. Pardo, and J. Samitier. *An intelligent detector based on temperature modulation of a gas sensor with a digital signal processor*. *Sensors and Actuators B*, Vol. 78, 2001.
- [16] A. Lee, B. Reedy. *Application of radiometric temperature determination methods to semiconductor gas sensors*. *Sensors and Actuators B*, Vol. 69, 2000.
- [17] H.D. Le Vine, “Method and apparatus for operating a gas sensor,” U.S. Patent 3906473, Sep. 16, 1975.

- [18]H. Eicker, "Method and apparatus for determining the concentration of one gaseous component in a mixture of gases," U.S. Patent 4012692, mar. 15, 1977.
- [19]L.J. Owen, "Gas monitors," U.S. Patent 4185491, Jan. 29, 1980.
- [20]G. N. Advani, R. Beard, and L. Nanis, "Gas measurement method," U.S. Patent 4399684, Aug. 23, 1983.
- [21]V. Lantto and P. Romppainen, "Response of some SnO₂ gas sensors to H₂S after quick cooling," *J. Electrochem. Soc.*, vol. 135, pp. 2550-2556, 1988.
- [22]S. Bulkowiecki, G. Pfister, A. Reis, A. P. Troup, and H.P. Ulli, "Gas or vapor alarm system including scanning gas sensors," U.S. Patent 4567475, Jan. 28, 1986.
- [23]W.M. Sears, K. Colbow, F. Consadori, "General characteristics of thermally cycled tin oxide gas sensors," *Semicond. Sci. Technol.* 4 (1989) 351– 359.
- [24]W.M. Sears, K. Colbow and Franco Consadori "Algorithms to improve the selectivity of thermally cycled in oxide gas sensors," *Sens. Actuators B*, vol. 19, pp. 333-349, 1989.
- [25]A. Vergara, E. Llobet, J. Brezmes, P. Ivanova, X. Vilanova, I. Gracia, C. Cané, X. Correig, "Optimised temperature modulation of metal oxide micro-hotplate gas sensors through multilevel pseudo random sequences," *Sensors and Actuators B* 111–112 (2005) 271–280.
- [26]A. Vergara, E. Llobet, J. Brezmes, X. Vilanova, P. Ivanova, I. Gracia, C. Cané, X. Correig, "Optimized Temperature Modulation of Micro-Hotplate Gas Sensors Through Pseudorandom Binary Sequences," *IEEE SENSORS JOURNAL*, VOL. 5, NO. 6, DECEMBER 2005.