Applying Neural Network for Calibration of SnO₂ Micro gas detector

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Abstract-A Design of a micro smell sensor based on semiconductor metal oxide method is presented. This sensor is able to recognize two different kinds of gas (CO and H₂) and will estimate the amount of dominate gas in the environment. The SnO₂ is employed as the key module of the sensor. A neural network calibration is applied to the sensor in order to identification of one of the two gases in an environment with complex combination of gases. The results vividly show that the sensor is able to approximate the amount of these two gases in the pool of gases.

Keywords: Micro smell sensor, Neural Network, error Backpropagation training, gas sensing

I. INTRODUCTION

The ability of gas detection has greatly attracted scientists' attentions in last decade. Gas sensors have many applications in various fields. Monitoring and control of the emissions in internal combustion motors and automobiles, measuring the amount of dangerous gases in laboratories and industries and controlling the amount of gases in domestic environments in order to assuring the safety of people are some of its application[1,2].

The experimental studies on surface of solids leaded the gas sensors to convert the chemical absorption of gas to some response signals [1-3]. The working principle of SnO_2 sensors is the chemical oxidation and reductions, by which some electrons will transport between the surface and the gas. It's would be note that micro scale heat transfer has a key role in this process. The process will cause generation of the response signals. [1-5]

One of the important tasks that gas sensors should accomplish is recognition of one specific kind of gas in an environment consisting of combination of gases. There are many ways by which the sensor could provide this ability. In this paper the Neural Network calibration is employed to learn the system how to identify one kind of gas.

The backpropagation training algorithm is applied to the sensor using 1000 predetermined data. After learning process the smell sensor demonstrated good response to the learned gases, and a showed the undefined mode for the environment without those gases.

II. PROPOSING OF SENSING MECHANISM

As it's discussed before, there are many sensing methods applied in smell sensors. Through these mechanisms the semiconductor oxides are one of the most common types. Simplicity of fabrication, non-contact mechanism and high reliability make this type of sensors on the center of industrial attention. The proposed SnO_2 sensor is able to identify two kind f different gases in an environment. This is a fair performance, as in many industries there is just need two determining and tuning of two kinds of gases. i.e. CO and H_2 in the emissions of internal combustion motors or H_2 in Hybrid car factories. Figure 1 shows the schematic view of different parts of this micro smell sensor.



Figure 1- schematic 2D and 3D views of micro smell sensor

The proposed sensor consists of six parts: wafer, heat and electricity insulator, heater, electrical insulator, sensing layer (SnO2) and electrodes. The main part of sensor is microhotplate, which generates proper heat to activate the sensing layer. Dimensions, material and properties of this layer should satisfy the amount of activation heat of sensing layer. In suggested sensor an aluminum layer is applied as the heater. The electricity and heat insulator should isolate the heater from its surrenders. Silicioum is employed to achieve a good insulator. It's worthy to note that the amount of wasted heat by insulator is calculated and added to activation amount which should be generated by heater.

The electrical insulator layer should have a property in hindering electricity in spite of high conductivity for heat. In order to satisfy this need, Si_3N_4 with large heat conductivity and electrical resistance is chosen.

The sensing layer will be activated in 520 $^{\circ}$ C, and by absorption of analyte its electrical resistance will change. Figure 2 shows the schematic of analyte molecules absorption to the sensing layer.



Figure 2- Schematic of analyte absorption to the sensing element As it is shown in figure 2, analyte molecules are absorbed by preheating of sensing element. By molecular reaction of analye ad SnO₂, amount of free electrons of sensing layer will change and therefore the conductivity of layer will face a change. Applying two electrodes into the sensing element is to measure variation of electrical resistance of sensing layer. In order to this, the electrodes are chosen to be gold. In this case, the electrodes resistance is very low, thus by changing conductivity of sensing layer the current of electrodes will change. Variation of current is the main item in determining the amount of variation in conductivity of sensing element. Finally it could determine the amount of analyte in environment.

III. MODELING OF CONDUCTIVITY VARIATION IN SNO2

Electrical conductivity in semi conductors is dependent to free electrons and their ability to movement. The electrical conduction σ is defined as below [14]:

$$\sigma = q \cdot \left(n \cdot \mu_n + p \cdot \mu_p \right) \tag{1}$$

Where q is charge, n is density of free electrons and p is density of gaps. μ_n and μ_p are electrons movement and gaps movements, respectively.

Poisson principle expresses an equation for *p*:

$$\rho(x) = q \left[N_d^+(x) - n_s(w) \right] \tag{2}$$

In this equation q is electron charge; N_{+d} is density of absorbed analyte to the surface and n_s is density of free electrons in depth of w [16].

The surface coating parameter in a constant temperature condition is given as [16]:

$$\Theta(T,p) = \left(\frac{p}{p_0(T) - p}\right) \cdot \left| \frac{c(T)}{1 + \left(\frac{p}{p_0(T)}\right)(c(T) - 1)} \right|$$
(3)

In this equation, p and p_0 are equilibrium pressure and saturated pressure in temperature of T, respectively. c(T) is Bit constant which is defined below [16]:

$$c(T) = \exp\left(\frac{\varepsilon_a - \varepsilon_L}{k_B \cdot T}\right) \tag{4}$$

Where ε_a is actual heat of analyte molecules and ε_L is equal heat of these molecules. As these two parameters are very close to each other, c(T) is assumed to be unit, and equation(3) will be written in a more simple shape.

Based on physical chemistry principles on semiconductor oxides, the electrical resistance of semiconductor oxide is written in equation (5) as a function of θ [17]:

$$\frac{R(t)}{R(0)} = \exp\left(Z\Theta_0^2\left(\left(1 - \frac{\eta}{\Theta_0} \frac{1 - \exp\left(-\frac{t}{\tau}\right)}{1 - \eta * \exp\left(-\frac{t}{\tau}\right)}\right)^2 - 1\right)\right) \quad (5)$$

In this equation θ_0 is initial coating; τ is constant of response time. η and η^* are chemical properties which are dependent to the analyte and the kinetics of chemical reaction. The parameter of Z in equation (5) is defined as [17]:

$$Z = \frac{eV_{b\max}}{k_B T} \tag{6}$$

In this equation, e is energy of electron, $V_{b max}$ is activation energy of free electrons and K_{b} is Boltzman constant.

IV. DIMENSIONAL AND FUNCTIONAL PROPERTIES OF MICROSENSOR

The three dimensions of each layer have been shown in figure (3). The amount of each parameter is presented in table I.



Figure 3- schematic of micro smell sensor

Table I- dimensional properties of sensor (each parameter is written in microns)

in interons)						
L1	L2	L3	L4			
400	0.5	0.2	0.2			
D1	D2	t				
200	140	100				

Total heat generative power is 32.6 mW and 3.5 mW is wasted through the system. Thus, the thermal efficiency of sensor is 89.3%.

V. WORKING PRINCIPLE

The network is a Perceptron network with 18 input layers, 54 latent layer and 5 out put layers. Based on this network the matrix of **V** has 54 rows and 18 columns (54×18) and **W** has 5 rows and 54 columns (5×54). Figure 4 shows a schematic of the artificial network.



Figure 4-the schematic of the employed network

The input of network is feed by the output of smell sensor. For this purpose the output electrical signal of smell sensor is digitalized to an array of 18 discrete. The output of neural network is a 5 digit array in which the 3 left bits of array are related to the number of layer of the gas, and the other 2 bits indicate a code for the gas (analyte). For example if the output array is $(0\ 0\ 1\ 0\ 1)$ it means that the gas of A is recognized by the sensing element 1.

The entries of matrices V and W will change by applying the train algorithm till the error became converge to an amount smaller than E_{max} . Figure 5 shows the E_{rms} _ the error in training of neural network, with respect to the number of trainings on the entries of matrices V and W.



Figure 5- the variation of E_{rms} with respect to the number of trainings (K)

VI. TRAINING AND THE RESULTS

A. The behavior of network while sensing analyte A

In training process about 1000 prerecognized input signals was employed. Then the behavior of network under various kinds of inputs was studied. First, by applying the error backpropagation algorithm the best inputs for analyte A is determined. Figure 6 and table II show the best output signals of sensing element 1 and the real amount of analyte as the real.



Figure 6- the sensed amount of analyte A (best) and the real amount of the analyte in environment (real). Voltage is fixed and equal to 10 Volt.

Table II-	The	numeri	cal co	mpare	between	sensed	amount	of anal	yte 1	
		1								

in sensing element 1 and it's real amount in the environment				
The Sensed	[0.7564 3.2708 3.0642 3.7243 4.1386 3.6137			
amount of	1.0665 1.7163 0.2174 -1.5639 -2.3752			
analyte 1	-2.2915 -1.0041 -0.7643 -0.8030 -2.8495			
	-2.6973 -3.2063]			
The Sensed	[0.5269 2.9133 2.6271 3.5924 4.0060			
amount of	3.1786 0.9481 1.3116 -0.2412 -1.6790			
analyte 1	-2.4951 -2.3117 -1.0432 -1.08668990			

In the same way the sensing behavior of sensing element 2 to analyte A is studied.

B. the behavior of network while sensing analyte B

The error backpropagation is implemented to the smell sensor, and the sensing quality is studied in both sensing elements 1 and 2. The quality of sensing in element 1 is shown in figure 7.



Figure 7- the sensed amount of analyte B (best) and the real amount of the analyte in environment (real). Voltage is fixed and equal to 10 Volt.

E. The behavior of network while sensing analyte *C* (untrained analyte)

To study the behavior of network to an untrained analyte, the system is feed by gas C. As the matrices of network are not trained for this gas, the network will identify the gas in its range of ability. The result of identification for gas C is $z=[0.0028 \ 0.0016 \ 0.9968 \ 0.6743 \ 0.3283]$ but according to our database the correct output for this gas was $d=[1 \ 0 \ 1 \ 1]$.

It can be seen that the system has tried to identify the input analyte but couldn't identify it correctly.

VII. CONCLUSION

A micro smell sensor is supposed and the neural network calibration is implemented on the sensor. By applying the error backpropagation training algorithm, the micro smell sensor is able to recognize two different kinds of gases in an environment with a good estimation of their amount.

According to the results, the sensor has good adaptation with the analytes that has trained by them and for untrained gases the sensor has no good identification in the environment. In the case that analytes A and B are CO and H_2 in environments which need to control the pollution in certain amounts.

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