Pattern recognition using AC treatment for semiconductor gas sensor array

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Abstract

Semiconductor gas sensor using tin oxide as sensing material has been used to detect gases based on the fact that impedance of the sensing material varies when the gas sensor is exposed to the gases. This variation comprises of two parts. The first one is variation in resistance of the sensing material and the other is expressed in terms of the sensor capacitance variation. Normally, only variation of the sensor resistance is considered. In this paper, using AC measurement with a capacitor-coupled inverting amplifier circuit, both changes in the sensor resistance and variations in the sensor capacitance were investigated. These characteristics were represented as magnitude gain and phase shift of AC signal at a specific frequency after passing it through the sensor and the designed circuit. A two-stage artificial neural network, which utilized the information above, was employed to identify and quantify three combustible gases: methane, propane and butane. The network outputs were approximately proportional to concentrations of test gases with reasonable level of error.

I. Introduction

It is well known that both resistance and capacitance of semiconductor gas sensors change when gas molecules chemically interact with the sensing material. Figure 1 shows the equivalent circuit of a typical semiconductor gas sensor. Surface and bulk reactions with gas molecules lead to the changes in overall direct current (DC) and alternating current (AC) conductance that may contain frequency-dependent contributions from doped (1) or undoped (1'), bulk (2), three-phase boundary or contacts (3), and grain boundaries (4)^[1,2]. The equivalent circuit with different RC units can explain the frequency behavior.

Generally, people are just interested in the changes in resistance (or conductivity) of the gas sensor in order to determine sensitivity of the sensor to the gases. In this paper, AC input signal at a specific frequency and capacitor-coupled inverting amplifier $^{[3]}$ were used to examine the sensor resistance and capacitance variation. A capacitor-coupled inverting amplifier is shown in Figure 2. Capacitors must not be allowed to interrupt the bias current paths to the op-amp input terminals. This sometimes requires additional bias resistors, which can affect the circuit input impedance. Since capacitors have their highest impedances at the lowest signal frequency, all coupling capacitor values must be calculated at the desired lower cutoff frequency (f_1) . The impedance of coupling capacitors at f_1 is usually determined as one-tenth of

the resistance in series with them. The largest capacitor in the circuit is normally selected to determine \mathbf{f}_1 and in this case the capacitive impedance is made equal to the series-connected resistance.

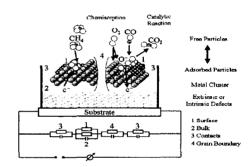


Fig. 1. Equivalent circuit of semiconductor gas sensor

The bias current to the op-amp inverting input terminal flows via resistor R_2 , so coupling-capacitor C_1 does not interrupt the input bias current. No resistor is included in series with the noninverting input terminal because a small dc offset is unimportant with a capacitor-coupled output. If it is desired to equalize the I_BR_B voltage drops, the resistance in series with the noninverting input should equal R_2 because R_1 is not a part of the bias current path at the inverting input terminal. The resistor values are determined as for direct-coupled inverting amplifier circuit. Then C_1 and C_2 are calculated to give $X_{C1} = R_1/10$, and $X_{C2} = R_3$ at f_1 , as in the case of a capacitor-coupled noninverting amplifier.

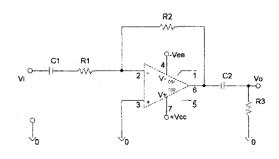


Fig. 2. Capacitor-coupled inverting amplifier.

II. Experiment

Four commercial semiconductor gas sensors were used. They are all Figaro sensors: TGS813, TGS842, TGS2611 and TGS2620. In the presence of a detectable gas, conductivity of sensor changes depending on the gas concentration in the air. TGS813 is high sensitive to a wide range of combustible gases. Both TGS842 and TGS2611 have high sensitivity to methane and low sensitivity to alcohol vapors. TGS2620 also has high sensitivity to a variety of combustible gases. The gas sensors were placed in a glass test chamber whose capacity is 3000ml.

Schematic of the designed circuit is shown in figure 3. Specifications of upper amplifier and below amplifier are the same. Gain and phase shift of the designed amplifier is about 4.7 and π respectively. AC impedance of gas sensor was observed to be flat in frequency range from 200Hz to 60kHz. Therefore, measurement has been conducted at 10kHz. Output signals (raw data) were measured using this circuit. Then gain and phase shift of the sensors were calculated from the raw data.

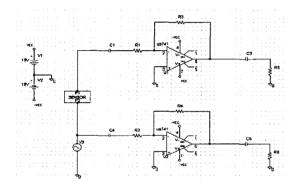


Fig. 3. Schematic of the designed circuit.

The gases used in this experiment were all combustible gases. They were methane, propane and butane. Gas concentrations were in the range of 1000-3000 ppm. Changing step was 500 ppm. Measuring procedure at each gas concentration was repeated 4 times so there were total 60 measurements or 60 patterns. All measurements were carried out at room temperature. The carrier gas was dry pure air.

III. Results and Discussion

Gain response of gas sensor is defined as ratio of amplitude of signal passing through upper amplifier and that of signal, which passes through the lower amplifier. At frequency of 10kHz, the output signals approximate

$$V_{lower} = V_{in} \times R_f/R_1$$

$$V_{upper} = V_{in} \times R_f/(R_1 + R_s)$$

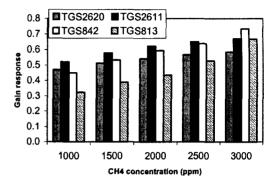
where R_f and R_s are feedback resistor and sensor's resistor respectively.

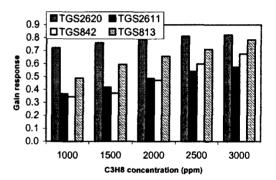
Then, gain response of the sensor is given as

$$Gain=V_{upper}/V_{lower}=R_1/(R_1+R_s)$$

Gain responses of gas sensors when the sensors were exposed to three combustible gases are depicted on figure 4. It is easy to recognize that the gain increases as gas concentration increases.

Because all the gases under the test are all reducing gases so the sensor resistance decreases when gas concentration increases. That why the gains of the sensors increase when gas concentration increases.





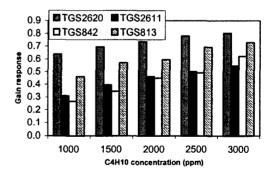


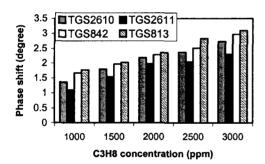
Fig. 4. Gain responses of gas sensors to methane, propane and butane.

The phase shift of each sensor was calculated from raw data. Phase shift data obtained when gas sensors reacted to CH_4 , C_3H_8 and C_4H_{10} are illustrated on figure 5. Similar to the sensor's gain, the phase shifts of the gas sensors increase as the gas concentration increases. It can be explained that when the gas concentration increases, the sensor capacitance increases. So the reactive impedance of the sensor decreases but in higher order than sensor resistance. Therefore, phase shift of gas sensor increases as gas concentration increases.

In order to explore the nature of the data and determine

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the linear separability of the sensor responses, principle component analysis (PCA) was performed on gain data, phase shift data or both gain and phase shift data. As shown on figure 6, PCA on the phase shift data could separate all of three gas clusters (CH₄, C₃H₈ and C₄H₁₀) but could not discriminate all gas sub clusters in each cluster. Meanwhile, PCA using the gain data could just distinguish methane from propane and butane. Performing PCA on both gain and phase shift data did not improve the result.



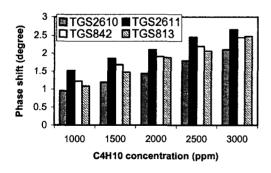


Fig. 6. Phase shift responses of gas sensors to methane, propane and butane.

To classify more precisely gas clusters with similar characteristics and to overcome statistical variances, multilayer neural network using error back propagation learning algorithm was utilized. A two-stage neural network^[4,5] was employed in order to identify and quantify three gases: methane, propane and butane (as shown on figure 7). In the first stage, network NN1 is responsible for identifying gases and is trained by phase

shift data. It has 4 input nodes, 8 hidden nodes and 3 output nodes. Each output node corresponds to one kind of gas. Missions of the last three networks (NN2 to NN4)in the second stage are to estimate the corresponding gas concentration. These networks had the same topology (4 input nodes, 6 hidden nodes and 1 output node) and were taught by using the gain data. All sub networks in the two-stage network were trained until mean square error (MSE) reduced below 0.0005 or the number of iterations exceeded 100000

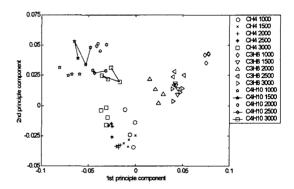


Fig. 6. PCA result on phase shift data.

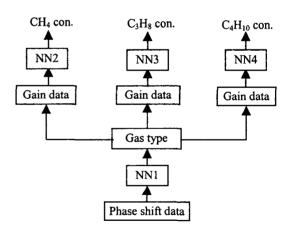


Fig. 7. Block diagram of two-stage network.

The training set for NN1 consisted of 45 patterns and the test set composed of other 15 patterns that were not used to train the network. In accordance with PCA result, predication rate was 100%. Once the gas was identified, its concentration was estimated with 3 networks (NN2 to NN4), one for each gas. To evaluate the quantitative analysis of gas patterns, mean absolute error (MAE) has been calculated.

It is given as

$$MAE_{j} = \frac{1}{N_{con}} \sum_{i=1}^{N_{con}} \left| test _out_{i}^{(j)} - test _tar_{i}^{(j)} \right|$$

where test_tar is the real concentration of gas, test_out is the predicted one, N_{test} is the number of testing patterns and j is the

notation of gas (i=1 \rightarrow CH₄, i=2 \rightarrow C₃H₈, i=3 \rightarrow C₄H₁₀).

Estimated gas concentrations and MAE values were given in figure 8 and table 1. All the gases were well identified and quantified with reasonable error level.

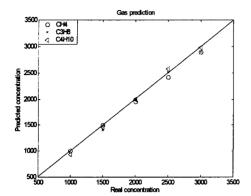


Fig. 8. Estimated gas concentrations.

Table 1. Mean absolute errors (MAEs in ppm)

Gas	Actual	Predicted	Difference
type	conc.	conc.	Difference
CH₄	1000	1000.9	0.9
	1500	1501.2	1.2
	2000	1947.4	52.6
	2500	2421.3	78.7
	3000	2892.6	107.4
	MAE		48.2
C ₃ H ₈	1000	988.4	11.6
	1500	1407.3	92.7
	2000	1990.7	9.3
	2500	2518.3	18.3
	3000	2900.7	99.3
	MAE		53.6
C₄H ₈	1000	926.8	73.2
	1500	1458.2	41.8
	2000	1997.6	2.4
	2500	2579.1	79.1
	3000	2980.4	19.6
	MAE		43.2

IV. Conclusion

Using AC signal treatment and designed capacitor-coupled inverting amplifier circuit, not only was resistance variation but also capacitance variation of semiconductor gas sensor investigated. These changes were represented as gain and phase shift of an AC signal that flow through the gas sensor.

When being exposed to combustible gases, semiconductor gas sensor has following response characteristic. As gas concentration increases, the gain response of semiconductor gas sensor increases, and also the phase shift response. These responses evidence that the resistance of semiconductor gas sensor is reduced, and the capacitance of semiconductor gas sensor is increased when gas concentration

increases.

Gain and phase shift responses of gas sensor array were used to train two-stage artificial neural network to identify and quantify three combustible gases (CH₄, C_3H_8 and C_4H_{10}). The classification rate at the first stage reached 100%. And the mean absolute errors of gas concentration prediction at the second stage were at reasonable level.

In conclusion we might say that the implemented system can be utilized for a higher number of gas sensors as well as for various gases.

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