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Application of an artificial neural network in the processing of output signals from a gas sensor with sol-gel-derived TiO_2 film

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TiO_2 thin film obtained by the sol-gel technique was used as the active layer in an electric sensor to distinguish the vapours of four volatile organic compounds: hexane, hexanol, cyclohexane and benzene. The measurements were performed at various temperatures of the sensing layer. Some of the output signals obtained from the sensor were characterized by low reproducibility, even within the data series obtained for the same gas. With the current design of the gas sensor, it was sometimes impossible to obtain a reproducible and stable output signal. Therefore, a neural network was used to pre-process the data. A bipolar transfer function of neurons was used as it had the shortest learning time of the network and produced the most stable results. The best results were obtained for a 4-4-4 topology of the neural network, where the input data were the values of the current at 440 and 360 °C when the sensor was exposed to a flow of air with or without organic vapours, with a 4-neuron hidden layer, and BE, CH, HL, HX outputs, each one associated with specific substance (benzene, cyclohexane, hexanol and hexane). The neural network was configured as a classifier recognizing four specific gases.

Key words: *smart sensor; volatile organic compound; sol-gel; artificial neural network; signal conditioner*

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1. Introduction

Thin titania films obtained by the sol-gel technique can be used as the active layers in electric sensors for various kinds of gases (e.g., CO, O_2, NO_x or vapours of volatile organic compounds [1–3]). By changing the precursors and solvents, choosing the method of layer deposition or setting the annealing temperature, a material with a controlled crystal structure, particle size, and surface area can be obtained. Unfortunately, the method may lead to low reproducibility and instability of the prepared material. It has been observed that the output signal of the sensor can exhibit low reproducibility even within the data series obtained for the same gas. To overcome this problem, pattern recognition (PARC) techniques can be applied in order to improve the quality of input data by means of data processing. Artificial neural networks (ANNs) are a promising technique which can be applied in chemical sensors [4–6].

In this paper, both the software and hardware implementation of a multilayer perceptron (MLP) are presented. The artificial neural network, complete with control software, was embedded into an analog microcontroller (8051-compatible core with integrated precision analog-to-digital and digital-to-analog converters). Considering its future use as a portable device, the system was designed to be compact and fully autonomic.

2. Experimental

The sensing titania thin film was prepared by means of the sol-gel method. The sol was obtained from titanium *n*-butoxide (TNBT) mixed with butanol and acetylacetone in the molar ratio of 1:20:2.3. After one hour of mixing in an ultrasonic bath, a small amount of distilled water was also added to the solution. All the compounds were further mixed together for 30 minutes and later left for 24 hours at room temperature.

The film was deposited with the modified dip coating technique [7]. An alumina plate with interdigital gold electrodes on one side and a Pt heater on the other side were used as a substrate. The part of the substrate with the electrodes and heater were immersed in the solution. Next, the sol was slowly poured out through a hole at the bottom of the container. After 10 min required for drying, the deposition was repeated three times to obtain a thicker film. The titania film was annealed in air for one hour at 600ºC with a heating rate of 10ºC/min.

The measurement system used in this project consisted of the following components: a gas sensor, a measuring chamber, a pure air generator, a chamber for vapour generation, a voltage supply, a measuring device, a rotameter, and a pump (the details can be found in [8]). The sensor was tested through the same sequential exposures. The sensing plate was exposed in turns to pure dry air and to air mixed with vapours of organic compounds. The exposure time was set at three minutes. To prepare the gaseous mixture, the stream of pure air flowed over a flask with liquid organic com-

pound thermostated at 50 ºC. The sensor response could be measured at various temperatures (in the range 275–440 ºC), depending on the voltage applied to the heater. The voltage supply was also connected to the sensor electrodes and changes of current during the exposure to gases were considered the response of the sensor.

3. Results and discussion

A thin film of titania with no cracks nor scratches was deposited on the alumina substrate. Some details about the film properties have been described earlier [9]. A typical response of the sensing layer for benzene and hexanol is shown in Fig. 1. The largest changes of current were usually observed for hexanol, while lower ones for hexane and cyclohexane, and the lowest for benzene.

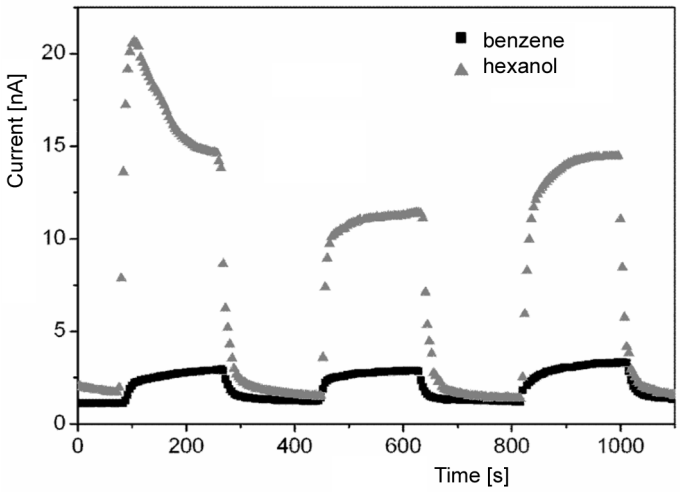

Fig. 1. The response of the sensor to the vapours of benzene and hexanol at 360 °C

Some of the output signals obtained from the sensor were characterized by low reproducibility even within the data series obtained for the same gas, as can be seen in Fig. 1 (the response to hexanol). The main reasons for this phenomenon could be: changes in the characteristics of the gas sensitive layer over time, changes of the sensor temperature during measurement, and variation of gas flow.

The sol-gel TiO_2 organic vapour sensor does not provide a direct output signal to distinguish between different gasses. It is also very hard to find an accurate mathematical model of the sensor [9]. In this work, after some investigations, an artificial neural network was chosen as the processing component for the sensor data.

There are two commonly used transfer functions of neurons: tanh() and sigmoid. Both are non-linear; tanh() is bipolar (–1…1 output range), while the sigmoid function is unipolar (0…1 output range). In our case, we observed that the bipolar transfer

function is the best choice since it ensures the shortest learning time of the network and the most stable results. The next step was to select the topology of the ANN. After screening (experimental data analysis), both dual- and triple-layer networks were selected for further experiments. Generally, the 1- or 2-neuron single hidden and 2-hidden-layer topology was not a good choice due to problems with local minima during learning. These networks were unstable and their learning time was relatively long.

Given the experimental data, the optimal network topology (with the shortest learning time and the lowest error) is 4-4-4 with min440, max440, min360 and max360 inputs, a 4-neuron hidden layer and BE, CH, HL, HX outputs (Table 1 and Fig. 2). The values for min440 and min360 represent the current at 440 or 360 °C when pure air is passed through the measuring cell and for max440 and max360 are the highest values of the current at 440 or 360 °C when the sensor is exposed to a flow of organic vapours. The outputs BE, CH, HL and HX are assigned to benzene, cyclohexane, hexanol, and hexane, respectively. During normal operation, only one output is activated, indicating a specific compound.

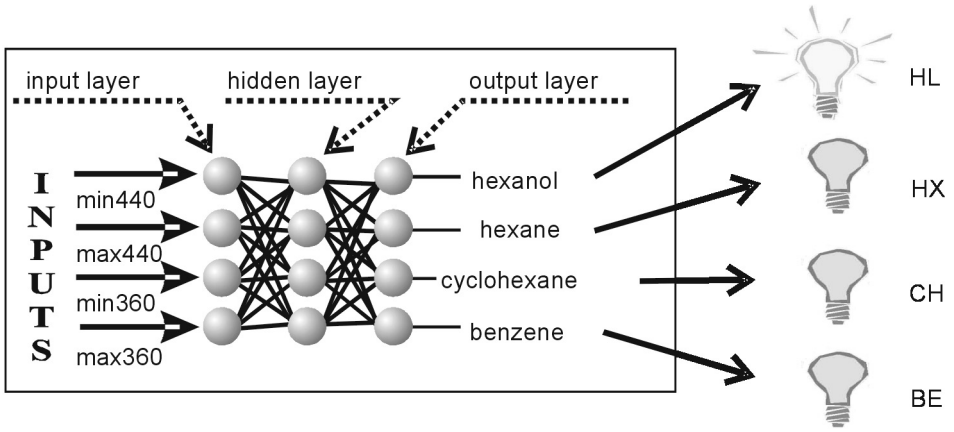

Fig. 2. Neural network structure

Table 1. Testing set – inputs and expected values (eBE, eCH, eHL, eHX)

min440	max440	min360	max360	eBE	eCH	eHL	eHX
16.6	36.7	1.23	2.84	**1**	0	0	0
15.5	36.3	1.23	2.84	**1**	0	0	0
10.4	59.7	1	3.2	0	**1**	0	0
10.4	63.8	1	2.9	0	**1**	0	0
11.5	67.2	1.4	30	0	0	**1**	0
11.4	83	1.4	30	0	0	**1**	0
8.2	108	1	49	0	0	0	**1**
8.3	107	0.3	34	0	0	0	**1**

Before the neural network processor can be used, it must be trained with the experimental data. The experimental data vectors were divided into 3 separate sets:

- training set (88 vectors),
- cross-validation set (12 vectors),
- testing set (8 vectors).

The final results for the 4-4-4 network are shown in Table 2. The results are almost perfect – no errors were found within the different testing sets. The network answers were stable and repeatable.

Table 2. Nnetwork outputs

BE	CH	HL	HX
0.99	0.00	0.00	0.01
0.99	0.01	0.01	0.00
0.01	**0.99**	0.01	0.00
0.01	**0.99**	0.01	0.01
0.01	0.00	**0.99**	0.00
0.01	0.00	**0.99**	0.01
-0.02	0.00	0.01	**0.98**
-0.03	0.01	0.01	**0.99**

As the topology of the network is fairly simple, it is possible to implement it in hardware as an embedded neural processor. The input signals are: $i(t)$, I, U, where $i(t)$ is gas sensor output current at 5 V, I, U – Pt heater power supply values. Knowing I and U, we can calculate both the power dissipated (P) and the resistance (R) of the heater. As R depends on the heater temperature, T can be measured directly on-sensor without additional components. By means of the MOSFET power transistor, the controller constantly controls the current (and power) dissipated in the sensor. As a result, we can maintain constant temperature on the sensor surface. The MOSFET transistor is also used to switch the heater on and off.

The bottom side of the sensor has a TiO_2 layer covering the gold electrodes. Given constant voltage supplied to the sensor (5 V), small current changes can be observed during temperature changes and for different organic vapours. The current is very low (0–100 nA), and it cannot be measured directly with the microcontroller ADC. As the time constant of the sensor is relatively high (over 180 s), a lock-in input amplifier can be used to achieve low noise, very small voltage and current offset, and high gain.

The Analog Devices AD8554 is a very good choice due to its offset voltage (V_{os}) of 1 μV, input offset drift of 5 nV/°C, input bias current (I_b) of 10 pA, single power supply and rail-to-rail inputs and outputs [10]. The controller hardware design is shown in Fig. 3. It consists of a power source, signal conditioners and an integrated data acquisition system based on the ADuC845 chip. The Analog Devices ADuC845 was chosen as it offers built-in precision analog-to-digital converters, digital-to-analog converters, and programmable gain amplifiers. 10 input channels can be configured either as single-ended or differential.

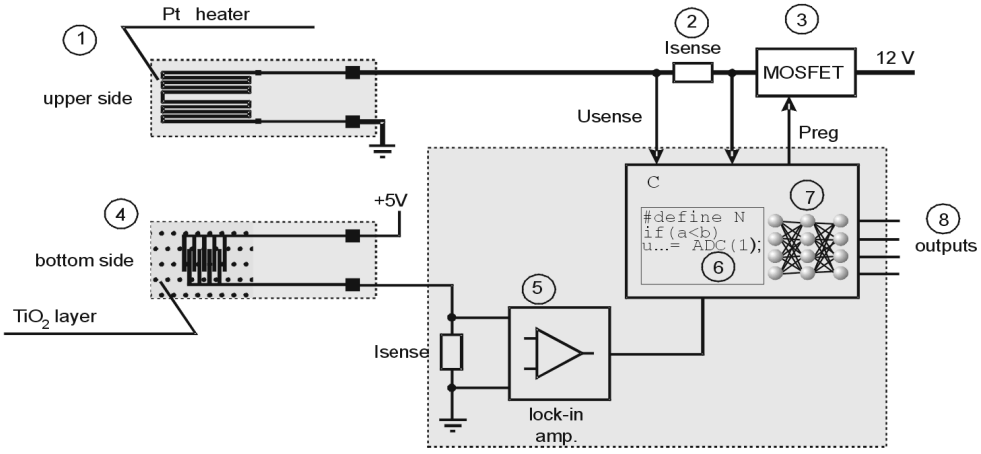

Fig. 3. Hardware design: 1 – Pt heater; 2 – series resistor for current sensing; 3 – MOSFET power transistor control of the curren, 4 – sol-gel TiO_2 coating sensing layer, 5 – lock-in precision amplifiers, 6 – control code power control, signal conditioning, 7 – ANN code, 8 – digital outputs

The device features are: two independent 24-bit ADCs, 10 analog input channels, 22-bit rms (19.5 bit p-p) effective resolution, offset drift 10 nV/°C, gain drift 0.5 ppm/°C (with chop enabled), 62-kbyte on-chip Flash/EE program memory, 12 MIPS @ 12 MHz, digital interfaces: UART, SPI®, and I2C® serial I/O, 34 GPIO pins, small outline dimensions (8×8 mm^2, Fig. 4).

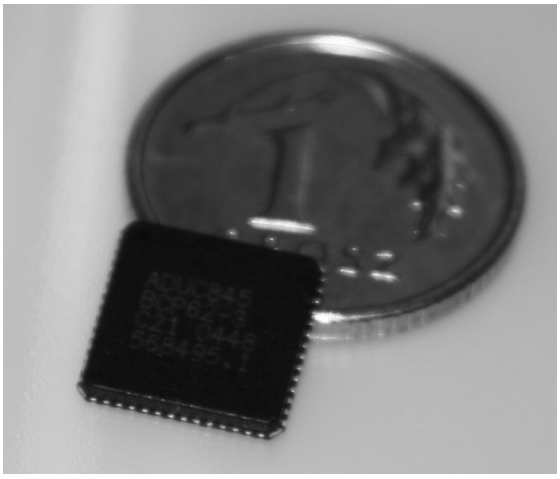

Fig. 4. Analog Devices' ADuC845 microcontroller

The combination of a gas sensor, a precision lock-in input amplifier, and 24-bit analog to digital converters provides a highly compact, accurate and cost-effective measurement system. The main advantage of using a microcontroller instead of pure ADCs is the ability to execute the code. The source code was written in C (both neural network and control code) [10].

The control code is responsible for time measurement, temperature stabilisation, and the preparation of input data for the neural network. After all data have been prepared, the second part of the code is executed. This part of the code is an implementation of a 3-layer perceptron consisting of 4-4-4 neurons. Within the code, the operation of the network is rather simple – each of the processing element is an adder with non-linear output function (tanh). The neurons are connected with synapses, represented by an array of floating-point numbers (neural network weights). As the ADuC845 does not provide a hardware implementation of a math co-processor, some of the calculations have to be software-emulated [10]. In our design, all of the network weights are calculated on a personal computer and hard-coded within the controller. The weights remain unchanged during the operation of the device.

The smart sensor design is very flexible – it can be used for different coatings, sensors and compounds [5]. The required changes can all be made in the software: the signal conditioner code and the weights (or topology) of the neural network. Each sensor-controller pair can be calibrated to achieve the best accuracy; long-term changes of the sensor properties can also be compensated.

The training time depends on the data sets and network structure; in our experiments, the range was between 3 and 10 seconds on an Intel Pentium 4 HT 3 GHz PC.

4. Conclusions

In modern sensors, especially organic gas sensors, there are often difficulties in interpreting output signals. In most cases, the raw output signal of the sensor depends on many factors and is not reproducible. The main goal is to obtain only meaningful results, while rejecting undesirable components.

This requires advanced data processing techniques, and an artificial neural network is a good choice. In practice, it is also very important for the sensor to be suitable for use outside of a laboratory environment. This can be achieved using a combination of a sensor, controller, and data processor.

We have presented a cost-effective, flexible design of a smart-sensor with an embedded artificial neural network. The effectiveness of the ANN in the classification of similar organic vapours is excellent, and the controller software can be easily adapted to other gas sensor designs and organic compounds.

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