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Wavelet transform and fuzzy ARTMAP-based pattern recognition for fast gas identification using a micro-hotplate gas sensor

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Abstract

It is shown that a single thermally-modulated tin oxide-based resistive microsensor can discriminate between two different pollutant gases (CO and NO_2) and their mixtures. The method employs a novel feature-extraction and pattern classification method, which is based on a 1-D discrete wavelet transform and a Fuzzy adaptive resonant theory map (ARTMAP) neural network. The wavelet technique is more effective than FFT in terms of data compression and is highly tolerant to the presence of additive noise and drift in the sensor responses. Furthermore, Fuzzy ARTMAP networks lead to a 100% success rate in gas recognition in just two training epochs, which is significantly lower than the number of epochs required to train the back-propagation network. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Discrete wavelet transform; Fuzzy ARTMAP; Micro-hotplate gas sensor; Tin oxide; Additive white noise; Sensor drift

1. Introduction

SnO_2 sensors are inexpensive and highly sensitive to a broad spectrum of gases, including atmospheric pollutants such as CO, NO_2 and H_2S [1–3]. However, well know disadvantages are their lack of selectivity and drift [4], which explain why these sensors are mainly used in low-cost alarm-level gas monitors for domestic and industrial applications [5]. A strategy to enhance selectivity consists of modulating the sensor's working temperature. When the sensor operating temperature is modulated, the kinetics of adsorption and reaction that occur at the sensor surface in the presence of atmospheric oxygen and other reducing or oxidising species are altered. This leads to sensor response patterns that are characteristic of the species present in the gas mixture [6–8]. Many examples of this approach can be found in the literature where the gas sensors employed can be conventional (e.g. TGS type [7]) or micromachined [9–12]. In most of these studies, the fast Fourier transform (FFT) is used to extract important features from the ac sensor signal together with a back-propagation neural network for predictive classification.

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In this work we show that the use of a novel feature-extraction technique like the discrete wavelet transform (DWT) that replaces FFT coupled to a Fuzzy adaptive resonant theory map (ARTMAP) neural network leads to better results. The performance of this technique in the presence of artificially generated noise and drift has also been studied. The DWT-based method was found to be highly tolerant to noise and sensor drift.

2. Experimental

2.1. Sensor

The device comprises an inert micro-hotplate substrate with a Pt heating resistor sandwiched between two thin silicon nitride layers and a pair of gold electrodes on top. The membrane thickness was about 0.6 μm and the active (hot) area of 250 μm × 500 μm. The gas sensitive layer was formed by depositing a Pd-doped SnO_2 paste onto the electrode area. Finally, on-chip annealing was performed at 450 °C in air (see [13] for further details). The micro-hotplate structure provides millisecond thermal response times and milliwatt power consumption required for hand-held units.

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Table 1
Single gases and binary mixtures measured

NO_2 (ppm)	CO (ppm)				
	0	20	40	80	130
0		✓	✓	✓	✓
10	✓	✓			
20	✓		✓		
40	✓			✓	
80	✓				✓

2.2. Measurements

Different concentrations of CO, NO_2 and their binary mixtures were tested (see Table 1 for details). A second set of NO_2 measurements was carried out 1 month later.

A sinusoidal voltage was applied to the heating resistor of the micro-hotplate sensor. The frequency was set to 50 mHz and the amplitude was adjusted to obtain a temperature variation from 243 to 405 °C. The circuit that drives the resistive heater (nominally 200 Ω) is shown in Fig. 1 [11]. Fig. 2 shows a typical dynamic response of the SnO_2 sensor in 20 ppm of CO. The sampling rate was set to 1.25 samples/s.

3. Results and discussion

At first, the pattern recognition system applied consisted of either an FFT or wavelet analysis coupled with principal component analysis. While the latter technique was used to classify response patterns (i.e. to establish the discrimination ability of the sensor), FFT and wavelet analyses were used to extract important features from the sensor response transients.

3.1. Fourier analysis

A 3750-sample FFT of every response transient was obtained (see Fig. 3). The FFT was calculated over a significantly large number of samples (150 periods of the signal) for the definition of the harmonic peaks to be good.

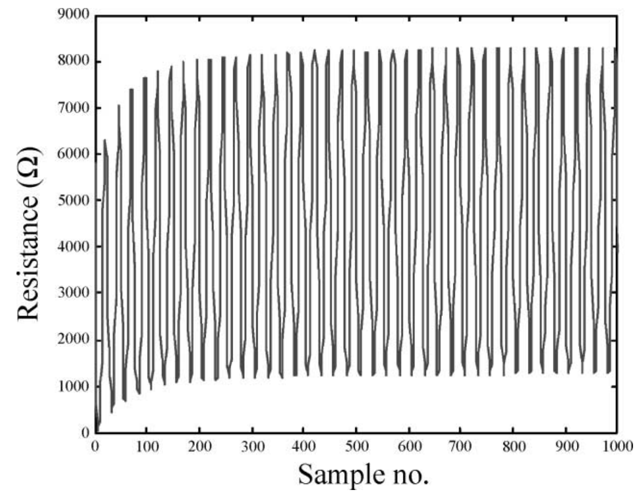

Fig. 2. Response transient corresponding to 20 ppm of CO in air.

Fig. 3 shows that peaks appear at multiples of sample no. 150 (e.g. 150, 300, 450, 600, etc.) this can be related to frequency f_0 considering the following equation:

$$f_0 = \frac{\text{sample no. of 1st peak}}{\text{total no. of samples}} \times \text{sampling rate} \quad (1)$$

Therefore,

$$f_0 = \frac{150}{3750} \times 1.25 = 50\,\text{mHz} \quad (2)$$

which is consistent with the frequency of the excitatory signal input to the sensor heating resistor. The higher harmonics in the FFT appear due to the non-linear characteristics of the sensor response.

The objective of this work was to discriminate between the different gases and mixtures (qualitative analysis). Since the dc component of the FFT is heavily dependent on gas concentration, this coefficient was not used for identification purposes. Therefore, the values of harmonics 1–6 were used

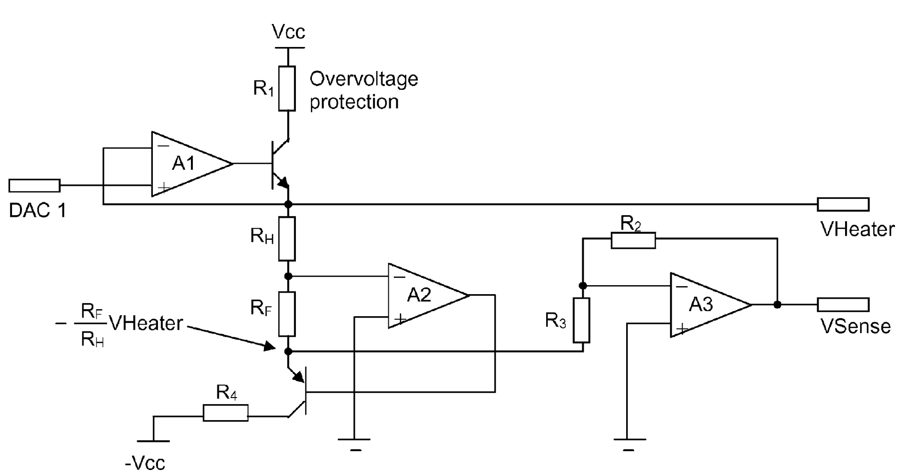

Fig. 1. Precision op-amp circuitry used to drive the sensor heating element.

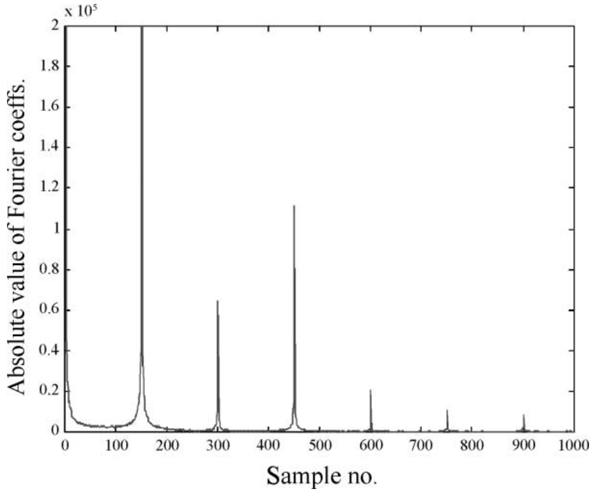

Fig. 3. FFT of a response transient corresponding to 20 ppm of CO in air.

in a principal components analysis. Data were mean-centred and the first two principal components accounted for 98% of variance in data.

Fig. 4 shows that a good separation was obtained. The second cluster for NO_2 (labelled NO_2 (2) in Fig. 4) corresponds to measurements performed 1 month later. The two NO_2 clusters are disjoint because after 1 month, the sensor response has drifted.

3.2. Wavelet analysis

Wavelet analysis provides an alternative way to Fourier analysis of breaking a signal down to its constituent parts. While Fourier analysis gives frequency information for the complete duration of the signal (temporal information is lost), wavelet analysis provides both frequency and temporal information. The shapes of the components of the decomposed signal depend on the shape of the analysing wavelet (there is a choice of several families). The goal of the DWT is to take the initial data sequence representing a chosen length of the discrete input signal $f(x)$ and convert it into a new sequence of real numbers $CW(x)$. These numbers define the vertical size of the wavelets at each of the set horizontal scales and positions in such a way that the addition of all the wavelets taken together, faithfully reproduces the original signal.

The wavelet expansion of $f(x)$ in $0 \leq x \leq 1$ can be written as:

$$f(x) = a_0\phi_x + a_1W(x) + [a_2 \quad a_3]\begin{bmatrix} W(2x) \\ W(2x-1) \end{bmatrix} + [a_4 \quad a_5 \quad a_6 \quad a_7]\begin{bmatrix} W(4x) \\ W(4x-1) \\ W(4x-2) \\ W(4x-3) \end{bmatrix} + \cdots + a_{2^j+k}W(2^jx-k) + \cdots \quad (3)$$

ϕ_x is the *scaling function*, $W(x)$ is a wavelet of scale 0, $W(2x)$ are wavelets of scale 1, $W(4x)$ are wavelets of scale 2, $W(8x)$ are wavelets of scale 3, and so forth. The higher the scale, the finer the detail and the more coefficients there are.

A single period of each measurement (28 samples) was used to perform wavelet analysis and the fourth order Daubechies (db4) was selected as analysing wavelet, because it is the first 'smooth' wavelet of the family. Fig. 5 shows a multi-level decomposition of a response transient.

The level 3 decomposition was selected, because it was found that wavelet coefficients ranging from 13 to 15 showed significant differences between the gases and mixtures to be discriminated.

A PCA was performed using coefficients 13–15. Data were mean-centred and the two first principal components accounted for 99% of variance in the data. Using only these three coefficients, an excellent separation was obtained (see Fig. 6). The dispersion within the NO_2 cluster is very low. This suggests that the effects of drift on the response

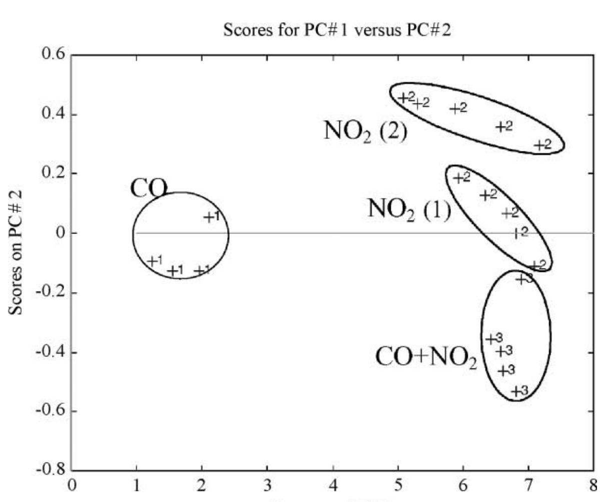

Fig. 4. PCA analysis using six coefficients of the FFT.

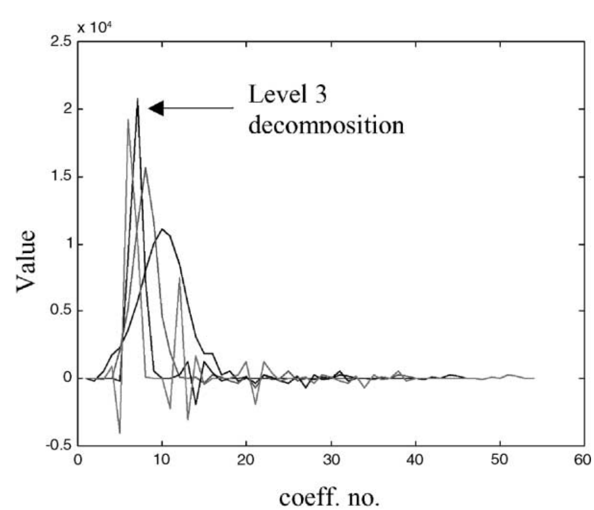

Fig. 5. Wavelet coefficients of a multilevel-decomposition of a typical response transient.

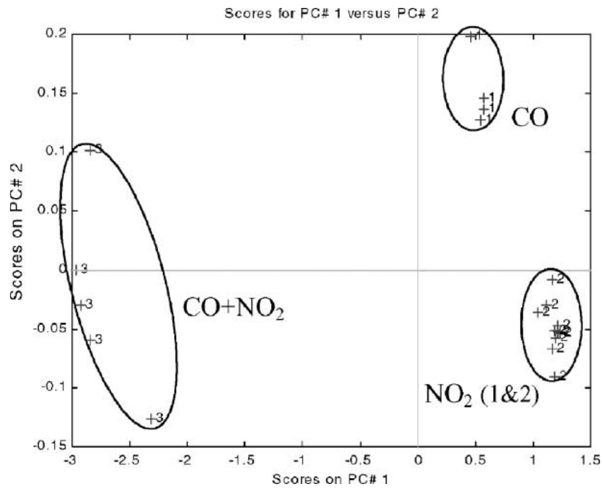

Fig. 6. PCA analysis using three wavelet coefficients.

transients have been removed by keeping a few wavelet coefficients.

3.3. Neural networks

Fuzzy ARTMAP is a self-organising and self-stabilising supervised classifier that shows generally superior performance in training compared with multilayer perceptron (MLP) [14,15] and more resilient to sensor drift. This is especially true when there is an uneven number of samples per category [16]. Therefore, in the second step a Fuzzy ARTMAP network was used for gas identification.

The network implemented for the classification of response features extracted by the FFT had six input neurones, because the first six harmonics were used. The number of output neurones was set to 3, since a 1-of-3 code was used to code the three different classes (i.e. CO, NO_2 and binary mixtures). Output neurones 1–3 represent the three different classes. For example, the identification of CO would yield a 100 at the output of the network, the identification of NO_2 would yield a 010 and finally, a binary mixture of CO and NO_2 would yield a 001.

The network used to classify response features extracted by the DWT had three input (coefficients 13–15 were used) and three output neurones, because the same 1-of-3 code was used.

A leave-one-out cross-validation method was used to estimate the success rate in classification. The networks needed just two training epochs and the number of category neurones (or neurones in the hidden layer) typically ranged between 3 and 5.

The Fuzzy ARTMAP neural network reached 90 and 100% success rates in recognition when six FFT coefficients and three wavelet coefficients were used as input vectors, respectively. These results, which are summarised in Table 2, are in good agreement with the PCA results shown in Figs. 4 and 6.

Table 2
Confusion matrices for the gas/mixture recognition with Fuzzy ARTMAP

	Actual		
	CO	NO_2	$CO + NO_2$
Predicted[a]			
CO	4	0	0
NO_2	0	9	1
$CO + NO_2$	0	1	4
Predicted[b]			
CO	4	0	0
NO_2	0	10	0
$CO + NO_2$	0	0	5

[a] 90% success rate with six FFT coefficients.
[b] 100% success rate with three wavelet coefficients.

3.4. Noise and drift rejection

To analyse how the different feature-extraction methods were able to deal with uncertainty and drift, which are key factors in any measurement system [17], noisy and drifting data were artificially generated.

To generate noisy data, uniformly distributed white noise was added with variances of 1, 5, 10, 20 and 50% to the experimental signals.

Fig. 7 shows the accuracies in classification attained by the fuzzy ARTMAP neural network in the presence of noise when the FFT and DWT were used as feature extractors. In this application, the DWT outperformed the FFT in the presence of noise. Fig. 8 shows a noisy signal corresponding to 20 ppm of CO with added white noise (variance of 20%) and the reconstructed signal using a third-level approximation and the db4 wavelet as analysing wavelet. Most of the high-frequency components, which correspond to noise, are removed in the reconstructed signal. This could explain the high resilience to noise of the DWT.

To generate drifting data two different cases were considered. In the first step the occurrence of long-term drift was simulated. This was done by adding a positive value to the mean of the signal and by altering its amplitude according to the following expression:

$$S_d = (S - \overline{S})(1 - d\alpha) + (1 + d)\overline{S} \quad (4)$$

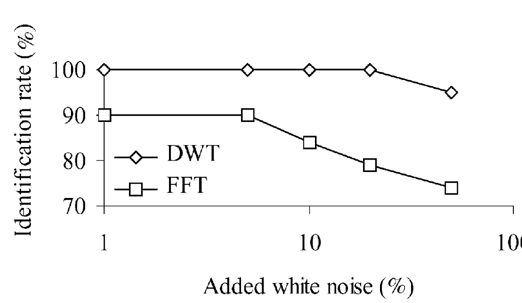

Fig. 7. Comparison of the accuracies in gas identification when the FFT and the DWT were used as feature extractors in the presence of added white noise.

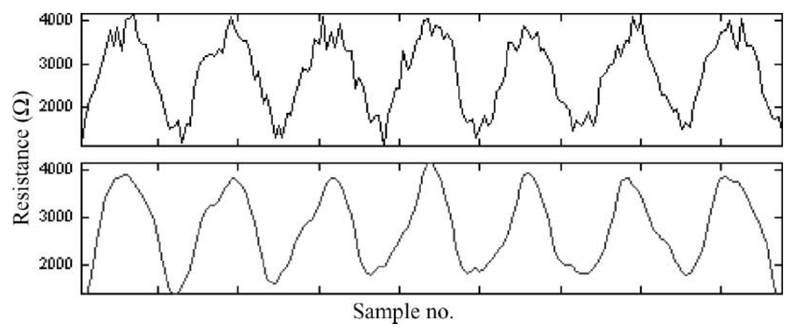

Fig. 8. Response transient corresponding to 20 ppm of CO with 20% added white noise (top). Reconstructed signal using a third-level wavelet decomposition (bottom).

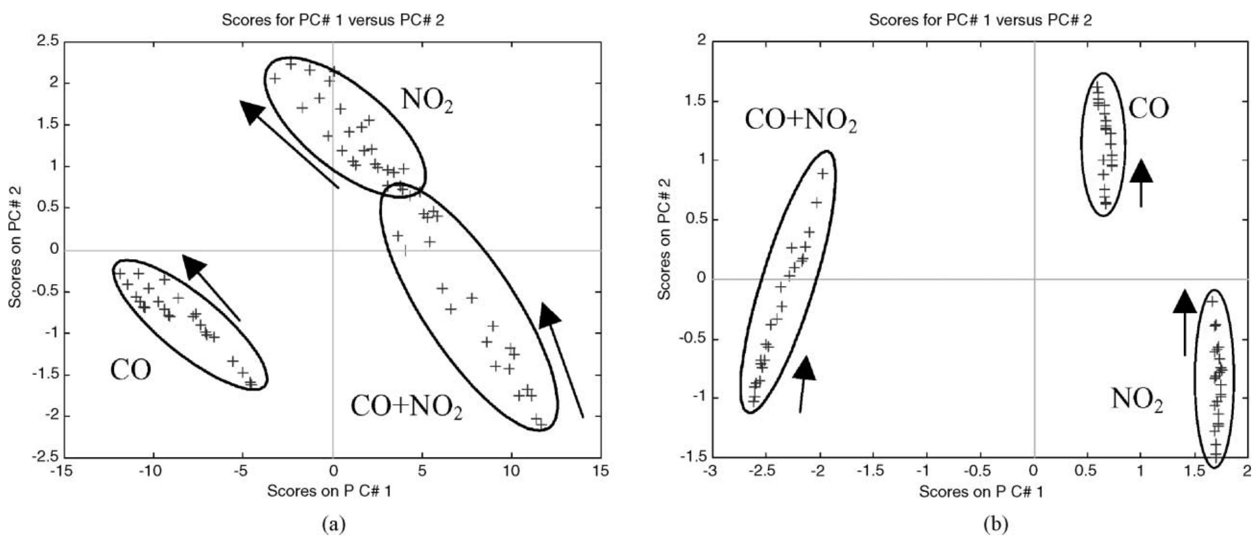

Fig. 9. Effects of long term drift on the resolving power using FFT (a) and DWT (b) to extract features from the sensor response. The arrows show drift direction and their length indicates the shift experienced within each cluster when drift increases from 0 to 50%.

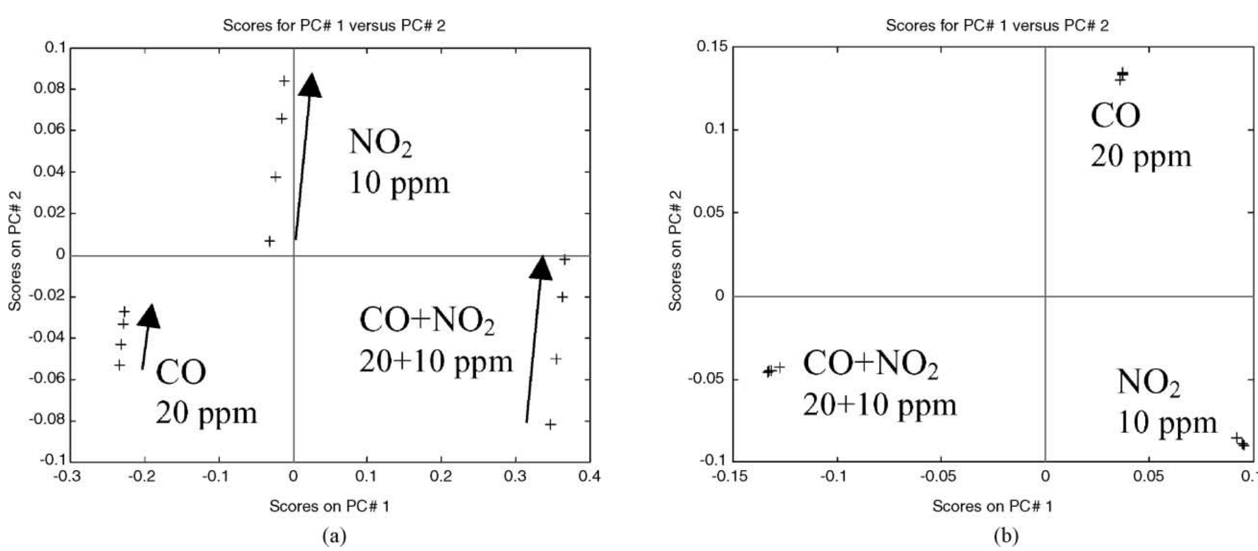

Fig. 10. Short-term drift effects. Using the FFT (a) and the DWT (b) to extract features from the sensor response. Drift increases linearly from 0 to 50% of the signal mean.

where S is the original signal, $\overline{S}$ its mean value, d is the drift constant (d is 1, 5, 10, 20 and 50%) and α is an arbitrary valued constant in the range $0 \leq \alpha < 1$. Eq. (4) was derived after analysing the differences in sensor response between the two NO_2 datasets —the second NO_2 dataset was measured 1 month later. The response signals in dataset #2 showed an increase in the mean and a moderate decrease in amplitude. The parameter α was set to 0.1.

Fig. 9 shows the results of a PCA carried out with the drifting data, using either the FFT or the DWT to extract important features from the sensor signals. The length of the arrows in Fig. 9 shows the importance of the shift in the score plots when d was altered from 0 to 50%. From Fig. 9 it can be derived that the DWT is highly tolerant to long-term drift.

In the second step the occurrence of short-term drift (i.e. effects in the present response of the sensor due to measurements in its recent past) was simulated. Short-term drift was generated by adding a positive linear ramp varying from 0 to half the mean of the signal. The duration of the ramp was set to 3750 samples of the signal (i.e. the number of samples used to compute the FFT). Fig. 10 shows the results of a PCA carried out with the short-term drifting data, using either the FFT or the DWT to extract important features from the sensor signals. Because short-term drift is a low-frequency process, it highly affects system performance when the FFT is used as feature extractor—the low harmonics of the FFT are essential for gas identification. On the other hand when the DWT is used, short-time drift effects are nearly removed. The fact that the low coefficients of the DWT, which correspond to the low-frequency contents of the signals are discarded, counteracts short-term drift.

4. Conclusions

The DWT was found to outperform a FFT in terms of data compression, drift rejection and tolerance to additive noise. The careful selection of appropriate wavelet scales counteracts drift, which is a low-frequency process, and reduces the effect of additive noise, which is associated to the high frequency content of the response signal. Furthermore, since it only requires a period of the response transient, wavelet analysis provides fast feature-extraction. Coupled with a Fuzzy ARTMAP network, which is trained in two epochs (e.g. typically more than two orders of magnitude less than the number of epochs required to train the back-propagation network) a 100% success rate was reached in the identification of CO, NO_2 and their mixtures. Therefore, the application of wavelet techniques to thermally-modulated resistive microsensors is attractive for low-cost handheld gas monitors.

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References

[1] P. Tasai, T. Chen, M. Tzeng, Tin oxide carbon monoxide sensor fabricated by thick-film methods, Sens. Actuators B 25 (1995) 537–539.
[2] T. Yoshida, N. Ogawa, T. Takahashi, Influence of NO and NO_2 composition on resistivity changes of SnO_2, J. Electrochem. Soc. 146 (1999) 1106–1110.
[3] V. Lantto, P. Romppainen, Response of some SnO_2 gas sensors to H_2S after quick cooling, J. Electrochem. Soc. 135 (1988) 2550–2556.
[4] P. Moseley, B. Tofield, Solid-State Gas Sensors, Adam Hilger, Bristol, 1987.
[5] J. Chou, Hazardous Gas Monitors, McGraw-Hill, New York, 2000.
[6] S.W. Wlodek, K. Colbow, F. Consadori, Signal-shape analysis of a thermally cycled tin-oxide gas sensor, Sens. Actuators B 3 (1991) 63–68.
[7] S. Nakata, S. Akakabe, M. Nakasuji, K. Yoshikawa, Gas sensing based on nonlinear response: discrimination between hydrocarbons and quantification of individual components in a gas mixture, Anal. Chem. 68 (1996) 2067–2072.
[8] P.K. Clifford, D.T. Tuma, Characteristics of semiconductor gas sensors: II. Transient response to temperature change, Sens. Actuators 3 (1983) 255–281.
[9] R.E. Cavicchi, J.S. Suehle, K.G. Kreider, M. Gaitan, P. Chaparala, Optimized temperature-pulsed sequences for the enhancement of chemically-specific response patterns from microhotplate gas sensors, in: Proceedings of the Conference of Transducers'95, Stockholm, 1995, pp. 823–826.
[10] A. Heilig, N. Bârsan, U. Weimar, M. Sweizer-Berberich, J.W. Gardner, W. Göpel, Gas identification by modulating temperatures of SnO_2-based thick-film sensors, Sens. Actuators B 43 (1997) 45–51.
[11] S. Al-Khalifa, J.W. Gardner, J.F. Craine, Sensors and their Applications, Vol. 8, IOP, Glasgow, UK, 1997, pp. 89, 94.
[12] L. Ratton, T. Kunt, T. McAvoy, T. Fuja, R. Cavicchi, S. Semancik, A comparative study of signal processing techniques for clustering microsensor data (a first step towards an artificial nose), Sens. Actuators B 41 (1997) 105–120.
[13] A. Heilig, N. Bârsan, U. Weimar, W. Göpel, Selectivity enhancement of SnO_2 gas sensors: simultaneous monitoring of resistances and temperatures, Sens. Actuators B 58 (1999) 302–309.
[14] G. Carpenter, S. Grossberg, N. Markuzon, J. Reynolds, D. Rosen, Fuzzy ARTMAP: a neural network architecture for incremental supervised learning of multidimensional maps, IEEE Trans. Neural Networks 3 (1992) 698–713.
[15] G. Carpenter, S. Grossberg, J. Reynolds, A Fuzzy ARTMAP non-parametric probability estimator for non-stationary pattern recognition problems, IEEE Trans. Neural Networks 6 (1995) 1330–1336.
[16] E. Llobet, E.L. Hines, J. W Gardner, Fuzzy ARTMAP-based electronic nose data analysis, Sens. Actuators B 61 (1999) 183–190.
[17] J.W. Gardner, P.N. Bartlett, Performance definition and standardisation of electronic noses, Sens. Actuators B 33 (1996) 60–67.

Biographies

Eduard Llobet graduated in telecommunication engineering from the Universitat Politècnica de Catalunya (UPC), (Barcelona, Spain) in 1991, and received his PhD in 1997 from the same university. During 1998, he

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Julian W. Gardner did his BSc, PhD, DSc, Ceng, FIEE, and MIEEE. Professor Gardner joined the School of Engineering at Warwick in 1987. His research interests are microsensors, microsystems technology, electronic noses, intelligent sensors and multivariate data processing methods. He has previously spent 5 years in industry working first at AEA Technology Ltd. and later at Molins Advanced Technology Unit on instrumentation. At Molins he developed a novel opto-electronic sensor that has been packaged in the UK and US for implementation on high speed packaging machinery. In 1989 he received the Esso Centenary Education Award sponsored by the Royal Society and fellowship of engineering to pursue his research interests. He has published over 200 technical papers and is an author of five books. He had an Alexander von Humboldt Fellowship in Germany in 1994. He currently heads the Sensors Research Laboratory in the Centre for Nanotechnology & Microengineering at Warwick University and is professor of electronic engineering.

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