New pattern recognition system in the e-nose for Chinese spirit identification*

Hui Zeng(曾慧), Qiang Li(李强), and Yu Gu(谷宇)†

School of Automation and Electrical Engineering, University of Science and Technology Beijing, Beijing 100083, *China*

(Received 14 July 2015; revised manuscript received 31 August 2015; published online 20 December 2015)

This paper presents a new pattern recognition system for Chinese spirit identification by using the polymer quartz piezoelectric crystal sensor based e-nose. The sensors are designed based on quartz crystal microbalance (QCM) principle, and they could capture different vibration frequency signal values for Chinese spirit identification. For each sensor in an 8-channel sensor array, seven characteristic values of the original vibration frequency signal values, i.e., average value (A), root-mean-square value (RMS), shape factor value ($S_{\rm f}$), crest factor value ($C_{\rm f}$), impulse factor value ($I_{\rm f}$), clearance factor value ($CL_{\rm f}$), kurtosis factor value ($K_{\rm v}$) are first extracted. Then the dimension of the characteristic values is reduced by the principle components analysis (PCA) method. Finally the back propagation (BP) neutral network algorithm is used to recognize Chinese spirits. The experimental results show that the recognition rate of six kinds of Chinese spirits is 93.33% and our proposed new pattern recognition system can identify Chinese spirits effectively.

Keywords: new pattern recognition system, polymer quartz piezoelectric crystal sensor e-nose, principle components analysis (PCA), back propagation (BP) algorithm, Chinese spirit identification

PACS: 42.30.Sy, 43.60.Lq, 07.07.Df **DOI:** 10.1088/1674-1056/25/2/024201

1. Introduction

The polymer quartz piezoelectric crystal sensor based e-nose[1] is a machine olfaction device to identify and monitor a variety of chemical gases of interest. It can imitate human senses by using polymer quartz piezoelectric crystal sensor arrays and pattern recognition system. Recently the developments of the polymer quartz piezoelectric crystal sensor, a quality sensitivity sensor outputting vibration frequency signal values, significantly promoted the improvement of the e-nose technology.[2–4] However, the e-nose is still in the early stages of application.

An effective pattern recognition system in the e-nose is needed to distinguish among different kinds of frequency signal values of testing materials. In fact, researchers have proposed many pattern recognition systems to improve the identification performance of the e-nose in market. For example, Chang and Freeman,[5] and Chang *et al.*[6] modeled a mammalian neural olfactory system that was characterized anatomically by modifiable synaptic connections, and physiologically by the spatiotemporal interactions among neural ensembles under external inputs. Ekachai and Nagle[7] dealt with selecting sensors for e-noses to make a portable device with fast response time, small size and reduced cost. Zhang *et al.*[8] presented an on-line counteraction of unwanted odor interference based on pattern recognition for the first time. Zhang *et al.*[9] studied the concentration estimations of indoor contaminants for air quality monitoring in dwellings by using chaos based on an optimal artificial neural network integrated into their self-designed portable e-nose instrument. Pawel and Wojciech[10] presented two innovative systems based on the feed-forward and recurrent neural network used for qualitatively analyzing the specimens of different fruit teas. Kizil *et al.*[11] developed an artificial neural network (ANN) model to identify the Salmonella enterica in poultry manure, and the accuracy is 94%. Although many successful pattern recognition systems have been designed for the e-nose, they cannot be used for the polymer quartz piezoelectric crystal sensor based e-nose directly. This is mainly because the signals, captured by the polymer quartz piezoelectric crystal sensor array, are nonlinear, and the sensors have cross sensitivity to the testing materials. The existing pattern recognition systems designed for the e-nose cannot extract the characteristic information about the polymer quartz piezoelectric crystal sensor effectively, and they must be updated and improved.

In our previous work, Gu and Li[12] presented a new pattern recognition system based on moving average and linear discriminant analysis (LDA), which could be used to process the original signal values of the new polymer quartz piezoelectric crystal air-sensitive sensor system. But only three kinds of Chinese spirits could be effectively identified and the adaptability of the pattern recognition system needs to be improved. In this paper, we propose another pattern recognition system for the polymer quartz piezoelectric crystal sensor based e-nose. For the vibration frequency signal values of six kinds of Chinese spirits captured by the e-nose, the proposed new

*Project supported by the National High Technology Research and Development Program of China (Grant No. 2013AA030901) and the Fundamental Research Funds for the Central Universities, China (Grant No. FRF-TP-14-120A2).

†Corresponding author. E-mail: guyu@ustb.edu.cn

© 2016 Chinese Physical Society and IOP Publishing Ltd

pattern recognition system could distinguish from them effectively. The new polymer quartz piezoelectric crystal sensor based e-nose, assembled with the new pattern recognition system, provides us with a new method to distinguish among Chinese spirits.

2. New pattern recognition system

To identify different kinds of Chinese spirits, a new pattern recognition system for the polymer quartz piezoelectric crystal sensor based e-nose is presented. First, the vibration frequency signal values are obtained by the polymer quartz piezoelectric crystal sensor array. Then for each set of vibration frequency signal values, seven characteristic values are extracted and the principal components analysis (PCA) method is used to reduce the dimension of the characteristic values. Finally the back propagation (BP) artificial neural network method is used to identify different kinds of Chinese spirits.

2.1. Signal acquisition of Chinese spirits

In this paper, we use the novel polymer quartz piezoelectric crystal sensor array to obtain the signal data of Chinese spirits, which is composed of different kinds of affinity-type polymer quartz piezoelectric sensors and very sensitive to the liquor product material. As shown in Fig. 1(a), the sensor is composed of polymer coating, quartz piezoelectric crystal plate, and polymer coating. The sensor is a quality-sensitive sensor, and its resonance will be disturbed by adding or removing a small mass of the polymer coating due to the adsorption or desorption to the testing materials, respectively. The vibration frequency values will be captured due to piezoelectric property of quartz crystal plate. The photo of the polymer quartz piezoelectric crystal sensor is shown in Fig. 1(b). We can prepare different kinds of sensors via adhering different kinds of polymer coatings.

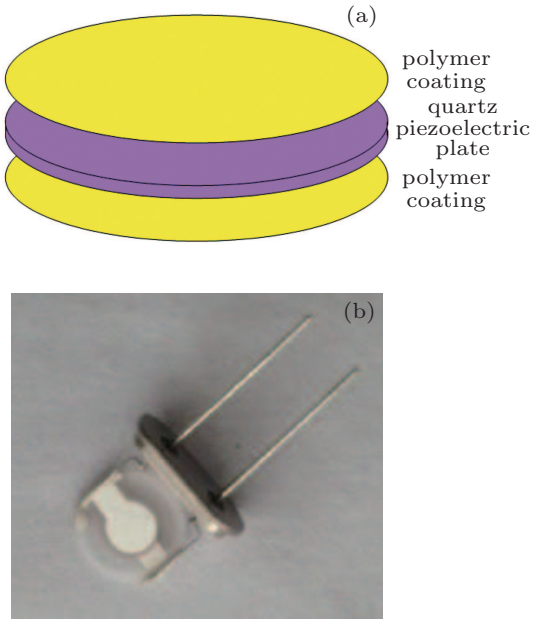


Fig. 1. (color online) (a) Photo and (b) structure of polymer quartz piezoelectric crystal sensor.

After studying the components of six kinds of Chinese spirits which are shown in Table 1, we select eight kinds of polymers to prepare eight kinds of polymer quartz piezoelectric crystal sensors. The selected polymers are shown in Table 2. As shown in Fig. 2, these sensors are assembled into an 8-channel sensor array. The vibration frequency signal values of the sensor array are captured 100 times per min.

Table 1. Six kinds of Chinese spirits.

No	Chinese spirit	Proof	Production date [year]	Origin
1	Shanxi spirits	106	2011	Xinghua village in Shanxi province
2	GuoJiao1573	106	2011	Luzhou in Sichuan province
3	Jiannanchun	106	2011	Mianyang in Sichuan province
4	Niu Lanshan	106	2011	Beijing in China
5	Wuliangye (spirit)	106	2011	Yibin city in Sichuan province
6	Jiugui Liquor	106	2011	Xiangxi autonomous prefecture, Hunan province

Table 2. Selected polymers for constructing quartz piezoelectric crystal sensors.

No	Sensor
1	PVC
2	polyamide
3	polyethylene + AgCl
4	polytef
5	AgCl
6	azithromycin
7	$CuCl_2$ + PE
8	$CuCl_2$ + AgCl + PE

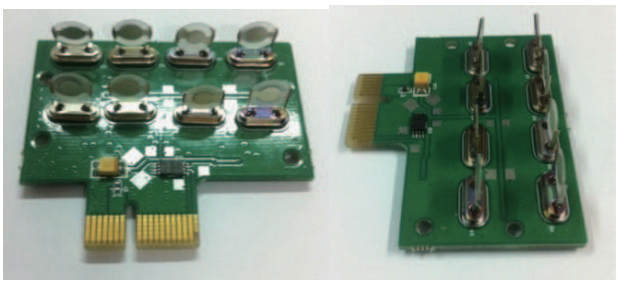


Fig. 2. (color online) Photo of the 8-channel sensor array.

2.2. Characteristic value extraction

As the changing trends of different kinds of vibration frequency signal values of Chinese spirits are similar, we extract seven characteristic values from the vibration frequency signal values to improve the accuracy of recognition. The seven characteristic values are average value (A), root-mean-square value(RMS), shape factor value ($S_{\rm f}$), crest factor value ($C_{\rm f}$), impulse factor value ($I_{\rm f}$), clearance factor value ($CL_{\rm f}$), and kurtosis factor value ($K_{\rm v}$). Our experimental results show that these characteristic values have rich distinctive information. The above characteristic values can be computed from the following equations:
for A,

$$\bar{x} = \frac{1}{N}\sum_{i}^{N} x_i; \tag{1}$$

for RMS,

$$x_{\rm rms} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} x_i^2}; \tag{2}$$

for $S_{\rm f}$,

$$S_{\rm f} = \frac{x_{\rm rms}}{|\bar{x}|}; \tag{3}$$

for $C_{\rm f}$,

$$C_{\rm f} = \frac{x_{\rm max}}{x_{\rm rms}}; \tag{4}$$

for $I_{\rm f}$

$$I_{\rm f} = \frac{x_{\rm max}}{|\bar{x}|}; \tag{5}$$

for $CL_{\rm f}$,

$$CL_{\rm f} = \frac{x_{\rm max}}{x_{\rm r}}; \tag{6}$$

for $K_{\rm v}$,

$$K_v = \frac{\frac{1}{N}\sum\limits_{i=1}^{N}(x_i-\bar{x})^4}{x_{\rm rms}^4}; \tag{7}$$

where x_i $(i = 1,\ldots,N)$ are the frequency values, and N is the number of the frequency values. Although the seven characteristic values have better distinctiveness than original signal values, our previous research work has shown that if we directly use the original signal values to distinguish among different kinds of Chinese spirits, the accuracy of recognition is low. So we need to extract some distinctive characteristic values for Chinese spirits' pattern recognition system.

2.3. Dimensional reduction of characteristic values

In order to reduce the computational complexity and improve the identification efficiency of the pattern recognition system, the PCA method is used to reduce the dimension of characteristic values. The PCA is a linear feature extraction technology based on data dimension reduction. It uses an orthogonal transformation matrix to project characteristic values from high-dimensional data space to low-dimensional data space, and it can convert characteristic values into a set of linearly uncorrelated values called principal components. Using PCA method, the raw signal values can be represented as a series of principal components. Let $X_1\ X_2\ \ldots\ X_n$ be the raw data, then the k-th principal component PC_k will be expressed as follows:

$$PC_k = a_{k1}X_1 + a_{k2}X_2 + \cdots + a_{kn}X_n, \tag{8}$$

where n is the dimension of the data, and $a_{k1}\ a_{k2}\ \ldots\ a_{kn}$ are the coefficients. The detailed description of PCA method can be found in Ref. [13]. With the PCA method, we can reduce the dimension of the Chinese spirit's characteristic values effectively. To improve the robustness of the recognition system, we use an average characteristic value of each kind of Chinese spirit to perform the PCA method and the first principal components are taken as the inputs of the classifier.

2.4. Chinese spirit recognition

In this paper, the BP neutral network algorithm is used to recognize six kinds of Chinese spirits in the new pattern recognition system. The BP neutral network is a multilayer feedforward network which can be trained by using error back propagation algorithm, and it is an effective method for classification. It can learn and store many input–output model mapping relations without using the descriptive equations of these relationships, and it can minimize the error sum of squares of the network by adjusting the network weights and thresholds.

In the BP neutral network, the number of the hidden layer nodes can be determined by the following equation:

$$l = \sqrt{n+m} + a, \tag{9}$$

where l is the number of the hidden layer nodes, n is the dimension of input data, m is the dimension of output data, and a is the adjusting constant from 1 to 10. The trained BP neutral network can be used to recognize different kinds of Chinese spirits.

3. Experimental results

In this paper, six kinds of Chinese spirits are used to testify the performance of the designed new pattern recognition system in the e-nose. First, the 8-channel polymer quartz

piezoelectric crystal sensor array is used for signal acquisition. For each kind of Chinese spirit, we capture vibration frequency signals for 2 min at room temperature in a clean room and 200 vibration frequency signal values are acquired. Such a manipulation is repeated 10 times. The signal values from 1st to 5th manipulation are used for training and the signal values from 6th to 10th manipulation are used for testing. Then six kinds of vibration frequency signal values of Chinese spirits can be acquired using the above method. Because of the limitation of length, a set of vibration frequency signal values of six selected kinds of Chinese spirits by sensor-1 are listed in Table 3, and their change tendencies are shown in Figs. 3–8. From Figs. 3 to 8, we can see that the changing trends of six kinds of Chinese spirits are similar.

Table 3. Frequency values of six selected kinds of Chinese spirits, detected by sensor-1.

No / Chinese spirit	Shanxi spirits	GuoJiao1573	Jiannanchun	Niu Lanshan	Wuliangye (spirit)	Jiugui Liquor
1	9996217	9996208	9996201	9995406	9995497	9996203
2	9996216	9996210	9996201	9995407	9995498	9996202
3	9996212	9996206	9996203	9995406	9995498	9996205
4	9996205	9996205	9996195	9995406	9995499	9996200
5	9996198	9996205	9996188	9995400	9995498	9996194
6	9996188	9996200	9996185	9995398	9995499	9996187
7	9996181	9996195	9996178	9995396	9995497	9996182
8	9996176	9996190	9996176	9995397	9995494	9996178
9	9996173	9996187	9996172	9995396	9995493	9996180
…	…	…	…	…	…	…
200	9996184	9996178	9996179	9995391	9995491	9996186

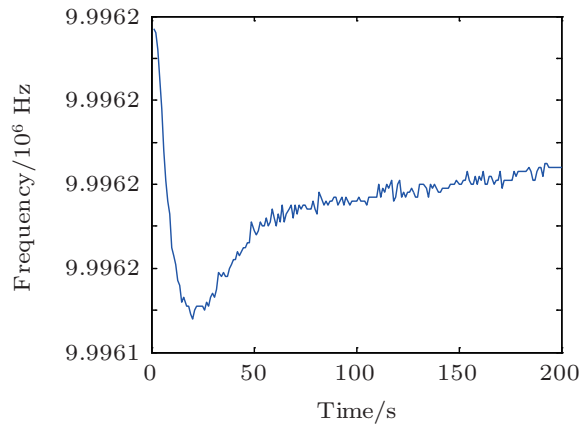


Fig. 3. (color online) Frequency values of Shanxi spirits.

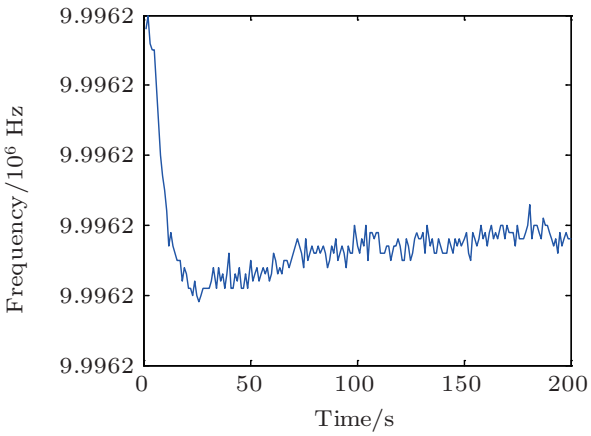


Fig. 4. (color online) Frequency values of GuoJiao1573.

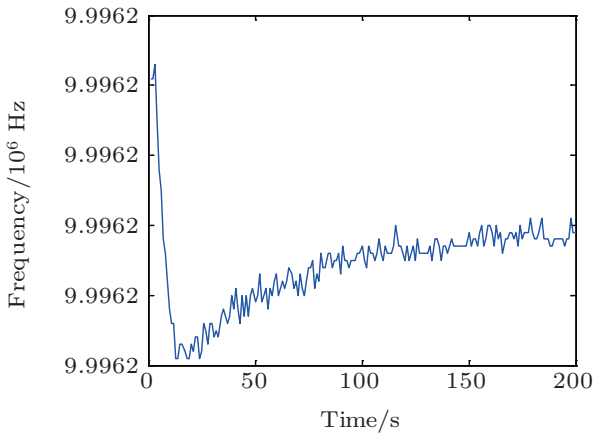


Fig. 5. (color online) Frequency values of Jiannanchun.

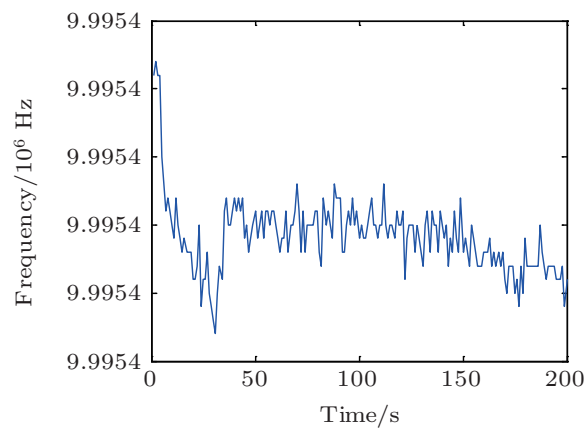


Fig. 6. (color online) Frequency values of Niu Lanshan.

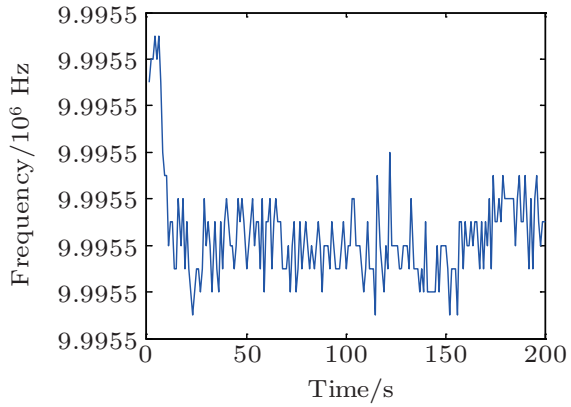


Fig. 7. (color online) Frequency values of Wuliangye (spirit).

For each set of vibration frequency signal values, seven characteristic values of six kinds of Chinese spirits are computed by using the signal values from 1st to 5th manipulation. Averaging each kind of characteristic value, we could obtain the characteristic values of six kinds of Chinese spirits. Taking the sensor-1 for example, the average characteristic values are shown in Table 4.

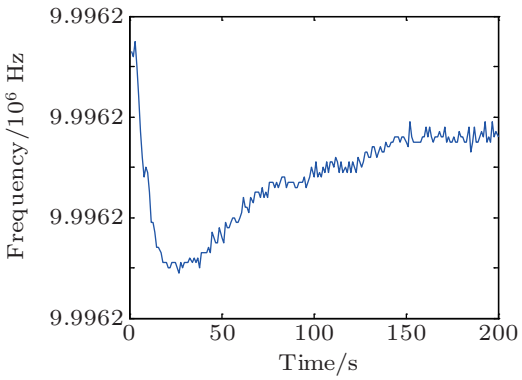


Fig. 8. (color online) Frequency values of Jiugui Liquor.

Table 4. Average characteristic values of six kinds of Chinese spirits (sensor-1).

Chinese spirit	A/Hz	RMS/Hz	S_f	C_f	I_f	CL_f	K_v
Shanxi spirits	9996200	9996200	1.0000	1.0000	1.0000	1.0004×10^{-7}	7.8691×10^{-24}
GuoJiao1573	9996200	9996200	1.0000	1.0000	1.0000	1.0004×10^{-7}	4.0899×10^{-24}
Jiannanchun	9996200	9996200	1.0000	1.0000	1.0000	1.0004×10^{-7}	4.1867×10^{-25}
Niu Lanshan	9995400	9995400	1.0000	1.0000	1.0000	1.0005×10^{-7}	5.6810×10^{-26}
Wuliangye (spirit)	9995500	9995500	1.0000	1.0000	1.0000	1.0005×10^{-7}	2.0544×10^{-26}
Jiugui Liquor	9996200	9996200	1.0000	1.0000	1.0000	1.0004×10^{-7}	2.1594×10^{-24}

As shown in Table 4, S_f, C_f, I_f, and CL_f have similar values, but A, RMS, and K_v have different values. These characteristic values indicate that the characters of the six kinds of Chinese spirits are similar, so we use the PCA method to extract more distinctive features. With the PCA method, we can obtain the first principal component of each kind of the seven characteristic values of Chinese spirits, and the results are shown in Table 5.

Table 5. Principal components of seven characteristic values.

Chinese spirit	Sensor-1	Sensor-2	Sensor-3	Sensor-4	Sensor-5	Sensor-6	Sensor-7	Sensor-8
Shanxi spirits	341.7683	–40.9658	–63.5901	–482.2617	119.7976	–302.9743	–14.7917	604.6131
GuoJiao1573	350.0796	21.5269	–36.6451	–503.0959	115.4177	–311.8485	–11.0455	594.4576
Jiannanchun	357.2256	–34.5113	–54.6155	–494.3843	127.4046	–324.9568	–25.2810	594.9893
Niu Lanshan	–761.2023	48.3277	82.5689	1007.1188	–250.7080	630.1365	43.2490	–1230.4733
Wuliangye (spirit)	–633.8962	36.34222	128.9848	960.9800	–231.1791	618.8752	16.3323	–1164.3036
Jiugui Liquor	346.0251	–30.71978	–56.7029	–488.3569	119.2672	–309.2322	–8.4631	600.7169

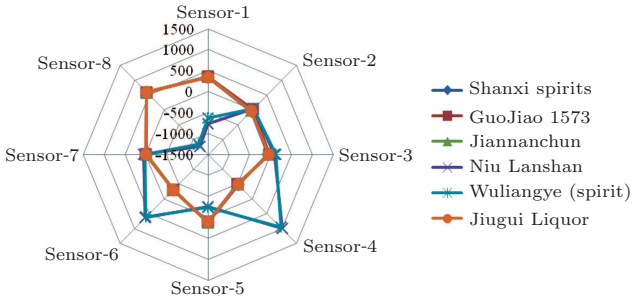


Fig. 9. (color online) Radar chart of six kinds of Chinese spirits' feature values of Chinese spirits.

As shown in Fig. 9, we insert the feature values of six kinds of Chinese spirits into a radar chart where each coordinate represents one kind of sensor. We can know that there are differences between different kinds of Chinese spirits. So we can use the principal components to represent the distinctive feature of each kind of Chinese spirit.

Finally, the BP neutral network is trained in the Matlab software. The number of hidden layer nodes is set to be 6, the maximum training time is set to be 1000, the minimum mean square error is set to be 1×10^{-8}, and the training goal is set to a 6×6 unit matrix. The training performance of the BP neutral network is shown in Fig. 10. The best training performance is reached at epoch 15. After training, the network weight and threshold of the BP neutral network can be com-

puted, and then the structure of the BP neutral network can be determined. The trained BP neutral network can be viewed as a classifier, and we use it to identify different kinds of Chinese spirits. In this paper, there are five testing samples for each kind of Chinese spirit, and the total number of testing samples is 30. The recognition rates are shown in Table 6. For Shanxi spirits, Jiannanchun, Niu Lanshan and Jiugui Liquor, the recognition rate of the new pattern recognition system is 100%. For GuoJiao1573 and Wuliangye, the recognition rate of the new pattern recognition system is 80%. The recognition of six kinds of spirits is 93.33%. These experimental results indicate that our proposed pattern recognition can distinguish among the six kinds of Chinese spirits effectively.

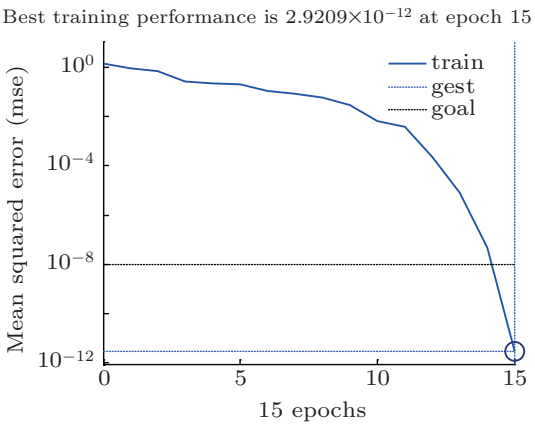


Fig. 10. (color online) Training performance of the BP neutral network.

Table 6. Recognition results.

Chinese spirit	Shanxi spirits	GuoJiao1573	Jiannanchun	Niu Lanshan	Wuliangye (spirit)	Jiugui Liquor	Total
Recognition rates	100%	80%	100%	100%	80%	100%	93.33%

4. Conclusions

This paper presents a new pattern recognition system to distinguish among six kinds of Chinese spirits by using a polymer quartz piezoelectric crystal sensor e-nose. First, seven characteristic values of six kinds of vibration frequency signal values of Chinese spirits, i.e., A, RMS, S_f, C_f, I_f, CL_f, and K_v are extracted. Then the PCA method is used to reduce the dimension of the characteristic values. Finally, the first principal components are used to train the BP neutral network and the trained BP neutral network is used to recognize Chinese spirits. The recognition results show that the recognition rates of six kinds of Chinese spirits are 93.33%. Our proposed new pattern recognition system provides us with a highly innovative method to recognize Chinese spirits.

References

[1] Gu Y and Li Q 2014 Proceedings 2014 *International Conference on Information Science, Electronics and Electrical Engineering*, pp. 1864–1867
[2] Gu Y, Li Q, Tian F F and Xu B J 2013 *Chin. Phys. Lett.* **30** 108101
[3] Gu Y, Li Q, Xu B J and Zhao Z 2014 *Chin. Phys. B* **23** 017804
[4] Gu Y and Li Q 2015 *Chin. Phys. B* **24** 078106
[5] Chang H J and Freeman W J 1996 *Neur. Netw.* **9** L-14
[6] Chang H J, Freeman W J and Burke B C 1998 *Int. J. Bifur. Chaos* **8** 321
[7] Ekachai P and Nagle H T 2008 *IEEE Trans. Instrum. Meas.* **57** 369
[8] Zhang L, Tian F C and Pei G S 2014 *Meas.* **54** 31
[9] Zhang L, Tian F C, Liu S Q, Guo J L, Hu B, Ye Q, Dang L J, Peng X W, Kadria C and Feng J W *Sensors and Actuators A: Phys.* **189** 161
[10] Pawel P and Wojciech M 2014 *Sensors and Actuators B* **192** 117
[11] Kizil U, Genc L, Genc T T, Rahman S and Khaitsa M L 2015 *Brit. Poul. Sci.* **56** 149
[12] Gu Y and Li Q 2014 *Chin. Phys. B* **23** 044213
[13] Jolliffe I T 2002 *Principal Component Analysis* (Springer Series in Statistics), 2nd edn. (Berlin: Springer)