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The estimations of ammonia concentration by using neural network SH-SAW sensors

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ABSTRACT

This paper presents the estimations of ammonia concentration by using neural network (NN) models. The shear horizontal surface acoustic wave (SH-SAW) devices coated with L-glutamic acid hydrochloride and polyaniline (PANI) film, respectively, were applied as the ammonia sensors. The data sensed by SH-SAW sensors were implemented by using different NN models. A reliable and superior neural network SAW identifier is expected to be found for effectively overcoming the interference of humidity in ammonia detection.

1. Introduction

Ammonia is commonly used in the refrigeration and fertilizer industries and is normally encountered as the gas with a pungent odor. Ammonia is also important in the formation and stabilization of ambient polluting aerosols, and these aerosol particles may cause disease in humans. Therefore, ammonia's widespread use and toxic nature bring a demand to monitor it quantitatively at its low concentration for avoiding health threat. Generally, humidity interference is often a serious problem of ammonia detection. For the medical application of detecting ppb concentration of ammonia, it is especially very important to identify the interference.

Shear horizontal surface acoustic wave (SH-SAW) have recently been demonstrated to respond the properties of analysis absorbed on the surface of SH-SAW devices directly. Obviously, SH-SAW devices are attractive for sensing applications due to their sensitive response, good reliability, small size, and low cost. The basic structure of SH-SAW sensor is made up of a SH-SAW device coated with a chemical interface that is sensitive to a specific element. The SH-SAW device is fabricated on a piezoelectric substrate, and the chemical interface is deposited between the input and output interdigital transducers (IDTs). The SH-SAW, emitted and received by a pair of input and output IDTs, propagates across the surface of piezoelectric substrate and generates both mechanical and electrical couplings between SH-SAW and chemical interface. The properties of chemical interface will be changed due to the interaction between interface and specific element. The interactions of SH-SAW and chemical interface then give the rise to phase velocity and attenuation responses of the acoustic wave. The shifts in velocity and attenuation are recorded by the frequency and insertion loss, respectively.

The chemical interfaces for detecting ammonia generally include metal-oxide and polymer films. Metal-oxide materials present a sensitive response to ammonia as they are operated at high temperature (100–300 °C). Rout, Hegde, Govindaraj, and Rao (2007) have reported the ammonia sensors based on ZnO nanoparticles and SnO_2 nanostructures sensitively responded to a wide range of ammonia concentrations (1–800 ppm). A sensor array consisting of discrete metal-oxides, i.e. SnO_2, ZnO, WO_3, CuO, and In_2O_3, has been successfully used to detect NO, ammonia, SO_2, and other gaseous pollutants (Tomchenko, Harmer, Marquis, & Allen, 2003). Pt doped SnO_2 materials have been shown high sensitivity to ammonia gas and stability (Wang, Wu, Su, Li, & Zhou, 2001). MoO_3 has been shown to be highly sensitive to ammonia, and the sensitivity depends on materials prepared processing (Prasad, Kubinski, & Gouma, 2003). The polymers are superior to metal-oxide films in their high sensitivity, low detection limit, and the ability in operating at room temperature. Most conducting polymers are sensitive to redox-active gases and organic vapors (Bai & Shi, 2007; Sadek, Wlodarski, Shin, Kaner, & Kalantar-zadeh, 2006; Zhang, Nix, Yoo, Deshusses, & Myung, 2006). Swelling effect, which can cause electrical resistance change, often occurs in conducting polymer layers. Polyaniline (PANI) is a conducting polymer and has a good electrical sensitivity to ammonia, so it has been used in electronic nose. S. Christie et al. have reported the application of electrochemically-prepared polyaniline films for the measurement of gaseous ammonia at telecom 1300 nm LED (Christie, Scorsone, Persaud, & Kvasnik, 2003). Based on the infra-

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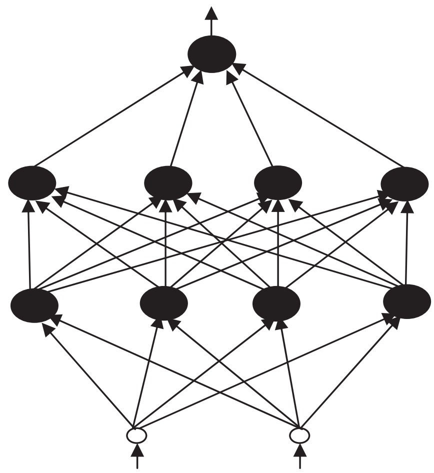

Fig. 1. The architecture of a four-layered neural network.

red spectra of L-glutamic acid hydrochloride, a reaction has occurred between the carboxyl group and ammonia to produce the ammonium salt of the carboxylic acid. Therefore, in our past researches, we studied the detection properties of SAW sensors to ammonia based on L-glutamic acid hydrochloride to ammonia in dry air (Shen, Hsu, Hsu, & Jeng, 2005; Shen, Hsu, Hwang, & Jeng, 2007; Shen, Huang, & Chuo, 2002). The detection limit of the L-glutamic acid hydrochloride sensor for ammonia was less than 0.90 ppm ammonia.

In this study, the estimations of ammonia concentration by using NN SH-SAW sensors were studied. Three different NN models were used as the estimators. A reliable and superior NN SH-SAW identifier is expected to be found for effectively overcoming the interference of humidity in ammonia detection. All NN models are composed of a four-layered feed-forward fully connected network which size is 2–4-4–1. The basic architecture of NN model is shown in Fig. 1. The detailed NN model and its learning algorithm are reported in Section 2. Section 3 presents the experiments of SH-SAW sensors. The simulations and results are presented in Section 4, and then a conclusion is made in Section 5.

2. Neural network models

As mentioned above, all NN models are composed of a four-layered feed-forward fully connected network. Three types of activation function, including sigmoid function, modified hyperbolic tangent function and n_s-level sigmoid function, are used in the nodes of NN models, respectively. Their math forms are expressed as follows.

$$f(x) = 1/1 + \exp(-x) \tag{2-1}$$

$$f(x) = a(1 - \exp(-bx))/(1 + \exp(-bx)) \tag{2-2}$$

$$sgm(x) = (1/n_s)\sum_{r=1}^{n_s}(1/(1 + \exp(-(x - \theta^r)))) \tag{2-3}$$

In each NN model, different layers could be composed of different types of node. But, each layer certainly is composed of the nodes having same activation function. To effectively distinguish the layers with different nodes, the layer formed by sigmoid function nodes is named SNN layer, the layer formed by modified hyperbolic tangent function nodes is named MNN layer, and the layer formed by n_s-level sigmoid function nodes is named QNN layer. According to the structure of neural layer, the learning rules of NN models could be summarized as follows (Purushothaman & Karayiannis, 1997; Shen, Huang, & Hwang, 2008; Weng, Chen, Huang, & Hwang, 2007).

We denote $S_j(k)$ as the desired output and $y_j(k)$ as the actual output of node j of the output layer on the presentation pattern k.

To SNN layer, the weight's adjustment is computed as follows.

For the output node j,

$$\Delta\omega_{ij}(k) \propto (S_j(k) - y_j(k))^*(y_j(k)(1 - y_j(k)))x_i(k) \tag{2-4}$$

For the hidden layer node j,

$$\Delta\omega_{ij}(k) \propto \sum_l \delta_l(k)\omega_{jl}(k)^*(y_j(k)(1 - y_j(k)))x_i(k) \tag{2-5}$$

where, $\Delta\omega_{ij}(k)$ is the weight adjustment between node j and its input $x_i(k)$ in the layer below. $\delta_l(k)$ is the error term feedback from node l in the layer above node j.

To MNN layer, the weight's adjustment is computed as follows.

For the output node j,

$$\Delta\omega_{ij}(k) \propto (b_j(k)/a_j(k))(S_j(k) - y_j(k))^*(a_j(k) + y_j(k))(a_j(k) - y_j(k))x_i(k) \tag{2-6}$$

$$\Delta a_j(k) \propto (S_j(k) - y_j(k))(y_j(k)/a_j(k)) \tag{2-7}$$

$$\Delta b_j(k) \propto (V_j(k)/a_j(k))(S_j(k) - y_j(k))^*(a_j(k) + y_j(k))(a_j(k) - y_j(k)) \tag{2-8}$$

where, $V_j(k) = \sum_i \omega_{ij}(k)x_i(k)$.

For the hidden layer node j,

$$\Delta\omega_{ij}(k) \propto (b_j(k)/a_j(k))\sum_l \delta_l(k)\omega_{jl}(k)^*(a_j(k) + y_j(k))(a_j(k) - y_j(k))x_i(k) \tag{2-9}$$

$$\Delta a_j(k) \propto (y_j(k)/a_j(k))\sum_l \delta_l(k)\omega_{jl}(k) \tag{2-10}$$

$$\Delta b_j(k) \propto (V_j(k)/a_j(k))(a_j(k) + y_j(k))^*(a_j(k) - y_j(k))\sum_l \delta_l(k)\omega_{jl}(k) \tag{2-11}$$

where, $\delta_l(k)$ is the error term feedback from node l in the layer above node j.

To QNN layer, the weight's adjustment is computed as follows.

For the node j,

$$\Delta\omega_{ij}(k) \propto ((1/n_s)\sum_{r=1}^{n_s} y_j^r(k)(1 - y_j^r(k)))^*\sum_l \delta_l(k)\omega_{jl}(k) \tag{2-12}$$

where, n_s is the number of levels and r is the number of jump points.

For the quantum interval adjustment, in each training epoch, we calculate the following outputs for each hidden node j.

$$\bar{h}_j = \sum_{i=0}^{n_i} \omega_{ij}X_i \tag{2-13}$$

n_i is the number of input signals.

$$h_j^r = \sum_{r=1}^{n_s} sgm(\bar{h}_j - \theta_j^r), \quad \tilde{h}_j = \frac{1}{n_s}\sum_{r=1}^{n_s} h_j^r, \quad \upsilon_j^r = h_j^r(1 - h_j^r) \tag{2-14}$$

Take the average values for each class, $\langle\tilde{h}_{j,Cm}\rangle$ and $\langle\upsilon_{j,Cm}^r\rangle$.

For mth class C_m,

$$\langle\tilde{h}_{j,Cm}\rangle = \frac{1}{|C_m|}\sum_{x_m, x_m \in C_m} \tilde{h}_{j,m} \tag{2-15}$$

and

$$\left\langle \upsilon_{j,Cm}^r \right\rangle = \frac{1}{|C_m|}\sum_{x_m, x_m \in Cm} \upsilon_{j,m}^r \tag{2-16}$$

where, $|C_m|$ denotes the cardinality of C_m.