Modeling polyvinyl chloride Plasma Modification by Neural Networks

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Abstract. Neural networks model were constructed to analyze the connection between dielectric barrier discharge parameters and surface properties of material. The experiment data were generated from polyvinyl chloride plasma modification by using uniform design. Discharge voltage, discharge gas gap and treatment time were as neural network input layer parameters. The measured values of contact angle were as the output layer parameters. A nonlinear mathematical model of the surface modification for polyvinyl chloride was developed based upon the neural networks. The optimum model parameters were obtained by the simulation evaluation and error analysis. The results of the optimal model show that the predicted value is very close to the actual test value. The prediction model obtained here are useful for discharge plasma surface modification analysis.

1. Introduction

In recent years, non-equilibrium plasma has been widely applied in industrial material treatment because it can offer a large number of active particles and is environment-friendly. Dielectric barrier discharge (DBD) is one effective way to produce atmospheric pressure non-equilibrium plasma and given special attentions due to the easy production of stable plasma. A large number of surface modification studies have been carried out by means of DBD technology [1]-[5]. But the combination influence of various discharge factors on surface properties have not been considered in these researches. As well known, it is very difficult to study the nonlinear character relationship between these factors and surface property for manual analysis. It also is not easy to build an analytic formula for the relation description. Consequently, there is a need to construct a appropriate model to analyze the above-mentioned relationship.

As for any relationship between input and output parameters, neural networks may learn complex information without any formulation because they have a great many neurons. The neurons have a architecture like that of the human brain and can complete parallel processing of data. The basic processors are interconnected with each other through the connection weights. A weighted sum of the input parameters of each neuron can be obtained after filtering with a sigmoid transfer function. The transfer function can raise the generalization ability of neural network by adding the degree of freedom [6]. A model based on neural networks technique has been built for processing semiconductor material[7].

In the paper, it is applied back-propagation algorithm neural networks for modeling the relationship between the discharge condition factors and surface hydropilh of polyvinyl chloride. The relation model is constructed by utilizing the toolbox of a business software named MATLAB. These
2. Experimental Design and Measurement

The data comes from the two parts of the experiment. The experimental data of one part are applied to train the neural network model. The experiments are performed in accordance with the U_{36}(4³) uniform design, where U indicates that the experiment is based on the uniform design, the number of 36 expresses total experimental frequency, 3 is the three experimental factors being considered, and 4 is the number of levels per factor. On the basis of reference [8], the 36 experiments can provide full messages on the 4³ complete experiments. Another part consists of 12 independent random experiments. The experimental results are used as testing data to evaluate the model. Here, the three discharge variables are applied high voltage, gas gap, and processing time. The applied discharge voltage includes 9kV, 10kV, 11kV and 12kV five levels. The time levels are 5s, 10s, 15s and 20s. The levels of discharge air gap are 0.5mm, 1mm, 1.5mm and 2mm.

A home-made plasma system is utilized to carry out polyvinyl chloride surface modification experiments in ambient air. Air plasma is produced between the two electrodes in case of that a high discharge voltage is connected to the upper metal electrode. In these experiments, discharge frequency is adjusted to 18 kHz. Polyvinyl chloride plastic film with 0.5 mm thick is cut into a lot of pieces which size is 20mm×20mm. The sample pieces are first cleaned five minutes by using hydrous alcohol, and then dried naturally in the air before modification. The contact angles of the sample surface is measured using 2ul distilled water drop in a commercial optical system. The result is the average of 10 contact angle measurements.

3. Neural Networks Structure Design

There are three neuronal layers in the common back-propagation neural networks (BPNN). They are input layer, hidden layer and output layer. The three discharge parameters as mentioned above are input to the neurons of input layer. The output data of output layer is consistent with the contact angle. Nonlinear operation is performed through the hidden layer neurons. As for error back-propagation (BP) learning algorithm, a single iteration comprises forward computation and backward-propagation two stages[9].

In the first stage, the output of the layer (k-1) is used to compute the weighted sum. A sigmoid function is used for filtering the sum. The neuronal output data of layer k is acted as the input data for the posterior layer l neurons. The whole active level s(ik) (m) for the kth layer neuron i is:

\[ s_{i}^{(k)}(m) = \sum_{j=0}^{p} w_{ij}^{(k)}(m) o_{j}^{(k-1)}(m) \]

Where \( o_{j}^{(k-1)}(m) \) is the (k-1)th layer j neuronal signal with the circulation m, \( w_{ij}^{(k)}(m) \) is the combination weight of the kth layer i neuron and the (k-1)th layer j neuron, and p is the kth layer neuron number. When \( j=0 \), then \( o_{0}^{(k-1)}(m)= -1 \), and \( w_{i0}^{(k)}(m) = \theta_{i}^{(k)}(m) \), where \( \theta_{i}^{(k)}(m) \) is the ith neuronal threshold in the kth layer. Thus, the expression of the ith neuronal output signal in the kth layer is as follows:

\[ o_{i}^{(k)}(m) = \begin{cases} 1 / (1 + \exp(-s_{i}^{(k)}(m))), & 1 \leq k < K \\ x_{i}(m), & k = K \end{cases} \]

Where in hidden layer, \( x_{i}(m) \) is the input vector ith element. When k=1, it means the first hidden layer. As for the last hidden layer, it is expressed by the letter K.

In the second stage, the weights can be updated for minimizing the error function. The error function can be described as the following representation:

\[ E_{i}^{(k)}(m) = 0.5(\hat{y}_{i} - y_{i}^{K}(m))^{2} \]

Where \( \hat{y}_{i} \) is target value of the ith element, and \( y_{i}^{K}(m) \) is the output of the ith neuron in the layer K. Error function is minimized according to the generalized delta rule based upon gradient descent method. The weight change delta is expressed as the following formula:
\[ \delta_{ij}^{(k)}(m) = [\hat{y}_j - y_j^{(k)}(m)]y_j(m)[1 - y_j(m)] \]  
\[ \delta_{ij}^{(i)}(m) = \alpha\delta_{ij}^{(k)}(m) + \sum_l \delta_{ij}^{(k+1)}(m)w_{ij}^{(k+1)}(m) \]  
\[ \Delta w_{ij}(m+1) = \eta\delta_{ij}(m+1)\sigma_j(m+1) \]  
\[ w_{ij}(m+1) = \eta\Delta w_{ij}(m+1) + \alpha\Delta w_{ij}(m) \]

In the first stage, the initial weights are random numbers. When the neuron networks calculate the last hidden layer outputs, the obtained deltas of each node in the output layer can update the weights and transmit the changes the input layer. The progress rules are as follows:

\[ \Delta w_{ij}(m+1) = \eta\delta_{ij}(m+1)\sigma_j(m+1) \]  
\[ w_{ij}(m+1) = \eta\Delta w_{ij}(m+1) + \alpha\Delta w_{ij}(m) \]

Here the iteration number is expressed by \(n\), the learning rate is denoted by \(\eta\) and the momentum is showed as \(\alpha\). The learning rate shows the weight rate for minimizing the error. The momentum \(\alpha\) is the ratio between the changes of the fore weight and the present weights.

4. Neural Network Model and optimization

The neural network does not need to design any mathematical model to deal with fuzzy, nonlinear and noisy data[10]. It can establish the model only depending on the input and output data. There are several key factors which can affect the model accuracy. They are the initial weight distribution, the allowable error and the neuronal number in the hidden layer. The initial weight is set in the range of \([-0.3, +0.3]\], and the same distribution is used in each simulation. It is enough for the allowable error set at 0.005 according to the engineering experiences. A neural network with single hidden layer is employed due to its solving any nonlinear mapping problem[11]. To optimize neural network, the amount of neuron of the hidden layer is changed from 2 to 20 step by step. The output layer has a single neuron and its output adopts the measured contact angle. A log-sigmoid function is acted as transfer function for the hidden layer. As for the output layer, a purlin linear function is put into use.

It is important to train BPNN for the model establishment. Since the web is learning to remember the proper patterns of problems, the training data should contain as many patterns as possible. The data obtained from the uniform design experiment are used to model the surface treatment. The first set of data obtained from the uniform experiment is applied for training BP networks. The learning rate used in BP network is 0.003. Training process is described as the following: first, two hidden layer neurons is used to train the BPNN. After training it is considered that the training results can meet the needs of the practical problems, if not, the neuronal number in hidden layer is increased for training again until the requirements are met. To optimize the BP networks model, the different predicted results are compared with different training parameters. If the root mean-squared error is the minimum error, the optimal model is obtained. The optimal thresholds and weights are stored and recorded in Table 1. It is known from the table that the structure of the optimal BP network model is 3-8-1.

| Hidden layer | Output layer |
|--------------|--------------|
| Thresholds   | Weights      | Thresholds | Weights  |
| 2.9153       | -0.13561     | 0.12936    | -0.10953 |
| 1.2068       | -0.50465     | 0.12048    | -0.008007 |
| -1.7738      | -0.6128      | -0.60871   | 0.23496  |
| 0.81244      | -0.35988     | -0.53892   | 0.093231 |
| 0.42259      | 0.64034      | 0.69225    | -0.23159 |
| -1.6486      | 0.21402      | -0.026457  | -1.1427  |
| 1.3845       | 0.17103      | -0.024621  | -0.90948 |
| -2.8149      | 0.10099      | 0.12775    | -0.15259 |

Table 1  The weights and thresholds of optimal BP model for PVC modification
5. Test results and Analysis

The optimal BP model estimated performance is shown in Figure 1. The predicted performance is analyzed by the absolute error, the mean absolute error, relative error, mean relative error and root mean-squared error.

![Graphs showing test results and analysis](image)

(a) The predictive results  
(b) The changes of absolute errors  
(c) The changes of relative errors

Fig.1. The predicted results and error changes of BPNN model

Figure 1(a) shows the comparison between the predicted value of the optimal and the practical measurement value of water contact angle. And it is in agreement with each other. The absolute error of calculation is in the scope of 0.061 to 0.887. It displays the mean absolute error is 0.4 as seen from Figure 1(b). In Figure 1(c), the relative error is 0.142 to 2.174 percent. The mean relative error is 0.888 percent. The root mean-squared error is 0.49 degree. All the results show that the model precision is high and in the permissible scope of engineering project. This shows that the proposed neural network has better performance for discharge plasma treatment forecast.

6. Conclusion

A BP neural network model has been constructed and applied for polyvinyl chloride surface modification with plasma technology. The modeling data used here come from two uncorrelated experimental group which is conducted by means of the uniform design experimental method. Three factors with four levels are used as experiment parameters in the present study. The optical structure of the model is three-eight-one. A great deal of training-and-testing for the optimization model display that the predictive accuracy is enough by using one layer as the hidden layer in treatment process. The model also has better predictive ability and can be applied to analyze the surface wettability modified by plasma technique. The final aim of the present study is for constructing a multi-function model for many materials treatment under different discharge plasma conditions. Such a model can enhance plasma treatment effect in industry and save more energy for our life.
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References

[1] N.Y. Cui, M.D Brown, Modification of the surface properties of a polypropylene (PP) film using an air dielectric barrier discharge plasma[J], Applied Surface Science, 2002 189(1-2) 31-38.

[2] B. Eliasson, U. Kogelschatz, Nonequilibrium volume plasma chemical processing[J], IEEE Transactions on Plasma Science, 1991 19(6) 1063-1077.

[3] A.D. Papalexopoulos, S. How, T.M. Peng, The barrier discharge: basic properties and applications to surface treatment[J], Vacuum, 2003 71(3) 417-436.

[4] G. Borcia, C.A. Anderson, M.D. Brown, Dielectric barrier discharge for surface treatment: application to selected polymers in film and fibre form[J], Plasma Sources Science and Technology, 2003 12(3) 355-344.

[5] C.Q. Wang, X.N. He, Effect of atmospheric pressure dielectric barrier discharge air plasma on electrode surface[J], Applied Surface Science, 2006 253(2) 926-929.

[6] C. Himmel, G. May, Advantages of plasma etch modeling using neural networks over statistical techniques[J], IEEE Transactions on Semiconductor Manufacture, 1993 6(2) 103-111.

[7] S.J. Ahong, G.S. May, D.-C .Park, Neural network modeling of reactive ion etching using optical emission spectroscopy data, IEEE Transactions on Semiconductor Manufacture, 2003 16(4) 598-608.

[8] K.T. Fang, C.X. Ma, Orthogonal and uniform experimental design, Beijing: Science Press, 2001. 93-103.

[9] M.T. Hagan, H.B. Demuth, M. Beale, Neural Network design, Beijing: China Machine Press, 2002. 306-406

[10] B. Kim, G.S. May, An optimal neural network process model for plasma etching[J], IEEE Transactions on Semiconductor Manufacture, 1994 7(1) 12-21.

[11] Y. Wada, and M. Kawato, Estimation of generalization capability by combination of new information criteria and cross validation, Proceedings of International Joint conference on Neural Networks, 1999 2 1-6.