Study on Mo process optimization of double glow plasma surface alloying based on BP neural network

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Abstract: On the basis of orthogonal experiment in double glow plasma surface alloying permeability Mo process, using the genetic algorithm of back propagation neural network (BPNN) GA, pole spacing and heat preservation temperature, holding time was studied, the source voltage and working pressure of process parameters on the double glow ion permeability molybdenum permeability layer thickness, the influence of the optimization of the double glow ion permeability Mo process test parameters. The predicted results are in good agreement with the actual test results, and the absolute coefficient (R²) is 0.964. The recommended optimal prediction method can get representative results for both the optimal and various penetration thickness predictions. This paper provides a new method for the selection of the optimum process scheme of double brilliance ionic infiltration Mo process.

1. Introduction

Double glow ionic metallization technology is a new surface modification technology for alloying on the surface of metal materials. It is an original national invention technology with independent intellectual property rights in China [1-2]. Its technology has a series of advantages, such as advanced, energy saving, controllable composition and a wide range of treatable materials.

Fig.1 shows the basic schematic diagram of double glow plasma metallization technology. The principle of double glow ion metallization is that a source composed of anode, cathode and elements to be permeated is arranged in a vacuum container. An adjustable DC power supply is arranged between the anode and cathode. The bias voltage can destroy the surface oxide film, activate the workpiece surface, and improve the temperature of the workpiece surface. It makes the elements easy to adsorb on the surface of the workpiece and is of great help to diffusion. An adjustable DC power supply is also provided between the anode and the source. When the vacuum degree of the furnace reaches a certain value, switch on two power supplies, so that the anode and cathode and anode and source respectively produce two layers of glow discharge, namely double glow. During ion
bombardment, seeping elements are sputtered from the source, and under the action of negative pressure, seeping elements bombard the workpiece surface and penetrate into the workpiece to form an alloy layer [3]. Ben et al. [4] used double-glow plasma infiltration technology to conduct molybdenum infiltration tests on the surface of Ti6Al4V alloy. The molybdenum modified layer is well combined with the substrate, and there is an obvious diffusion layer between the modified layer and the substrate. The thickness of the modified layer is about 30μm. The grinding performance is about 216 times higher than that before Mo infiltration treatment, showing excellent wear resistance.

![Image](image.png)

**Fig.1 Basic principle diagram of double-layer glow plasma metal infiltration technology**

The multi-layer forward neural network of error back propagation, proposed by Rumelhart, McClelland, etc. in 1986, has become the most widely used neural network. Its characteristic is that there is no feedback connection between neurons in each layer, only the neurons in the adjacent layer are connected, and there is no connection between the neurons in the layer [5]. The training process of the BPNN learning algorithm can also be simply summarized as follows: first initialize the weight \( W_{ji} \), the threshold \( \theta_j \), and then input the training samples, calculate the output state for each sample \( k \), get its error, and adjust the network layer according to the error back propagation. The weights and thresholds are adjusted repeatedly in this way until the network error \( E < \varepsilon_1 \) (\( \varepsilon_1 \) is the set error). After the sample training is completed, input the test sample. If the network error \( E < \varepsilon_2 \) (\( \varepsilon_2 \) is the test error) at this time, the network can be used for actual prediction. By establishing the BP neural network constitutive model of Ti-25Nb alloy, Ou et al. [6] studied the flow stress behavior of Ti-25Nb alloy under the conditions of 470-620℃ and 0.001-10s\(^{-1}\). The calculation accuracy of the model is high, with the correlation coefficient of 0.9996 and the relative error of 4.27%, which can accurately predict the flow stress behavior of Ti-25Nb alloy.

This paper takes the Shuanghui ion dosing Mo process experiment as the research object, establishes a three-layer BP neural network model, uses MATLAB software to simulate the sample signals of the neural network, and trains the neural network model. The selection of the best process parameters provides a new method. Taking the thickness of the infiltration layer as the target, the five process parameters that affect the thickness of the infiltration layer are used as input variables, and the function approximation function of the neural network is used to optimize the design to obtain the best process parameters. The calculated results are compared with the experimental results. Shows that the optimization results are accurate.

### 2. Materials and methods

#### 2.1. Materials and sample preparation

The base material is industrial pure iron, the size is: 30 mm × 10 mm × 2 mm. The source used a pure molybdenum plate with a purity of 99.99%. The size of the source plate is 70mm×45mm×5mm.

The source target material used in this study is a pure molybdenum plate with a purity of 99.99% and the size of plate is 70mm×45mm×5mm. Industrial pure iron is selected as the test matrix material,
the size is: 30 mm × 10 mm × 2 mm. Before experimenting with a vacuum furnace, we should polish the target and matrix materials. Then, using alcohol and acetone to clean the target and matrix materials by ultrasonic for about 20 minutes and finally dried the sample.

2.2. Methods

DGLT-15 type multifunctional ion chemical heat treatment furnace is used for Mo infiltration treatment. The auxiliary cathode adopts a rectangular carbon steel box with a size of 210 mm × 150 mm × 180 mm (length × width × height), and the sample and the molybdenum plate are suspended. In the auxiliary cathode, and add a cover plate to heat insulation. The working temperature of Mo infiltration is tested by WDL-31 photoelectric thermometer; the source voltage and working pressure are adjusted, and the infiltration process of heating and heat preservation is implemented. After infiltration of Mo, the sample is slowly cooled to room temperature along with the furnace.

The structure, morphology and thickness of the molybdenum alloy layer were observed with the German Zeiss Carl Zeiss Axio Scope A1 optical microscope and the German JEOL/JSM-5610LV scanning electron microscope.

3. Establish BP neural network prediction model

At present, in terms of prediction, BPNN mainly has problems such as over-fitting, poor generalization (prediction) stability, and difficulty in determining the network structure [7]. The predictive ability of BPNN is directly related to the question of whether it can be applied. Because there are too many factors that affect the thickness of the infiltrated layer in the double-glow ion molybdenum process, it is impossible to reflect the exact relationship between the process conditions and the thickness of the infiltrated layer through an accurate formula. Therefore, the BP neural network is established to learn the mapping relationship of a large amount of data through its own learning ability, so as to find the linear connection between the two. At the same time, based on the model already obtained, combined with the optimized process formula obtained by the orthogonal experiment, a better process formula can be found in a smaller range.

3.1. Data source and selection of training samples

BP neural network has very high requirements on samples, and not all input and output data can get ideal linear connection. Therefore, choosing true, reliable and reasonable data becomes the primary issue. The experiment selected by the orthogonal experiment design can fully reflect the law of the selected system. Although it reduces the number of experiments, the experimental data obtained can also fully reflect the internal relationship between various factors and indicators. General neural network models all use orthogonal experimental data as samples, because the combination of experimental factors is representative, and the results can be used to establish an efficient and reliable neural network. In this experiment, the orthogonal table is used to arrange the experiment, and the experimental data of the double-glow ion infiltration Mo process is used as the training sample of the neural network to establish the BP neural network. The input parameters are training samples, as shown in Table.1.
Table 1: Training neural network data sample

| Test Number | Electrode Distance/mm | Holding Temperature °C | Holding Time/h | Source Voltage/V | Working Pressure/Pa | Thickness Layer/μm |
|-------------|-----------------------|-------------------------|----------------|------------------|---------------------|--------------------|
| 1           | 15                    | 900                     | 3              | 800              | 25                  | 40.49              |
| 2           | 15                    | 960                     | 4              | 850              | 30                  | 60.97              |
| 3           | 15                    | 1020                    | 5              | 900              | 35                  | 78.05              |
| 4           | 15                    | 1080                    | 6              | 950              | 40                  | 82.2               |
| 5           | 20                    | 900                     | 4              | 900              | 40                  | 49.23              |
| 6           | 20                    | 960                     | 3              | 950              | 35                  | 51.04              |
| 7           | 20                    | 1020                    | 6              | 800              | 30                  | 84.97              |
| 8           | 20                    | 1080                    | 5              | 850              | 25                  | 89.58              |
| 9           | 25                    | 900                     | 5              | 950              | 30                  | 48.36              |
| 10          | 25                    | 960                     | 6              | 900              | 25                  | 60.22              |
| 11          | 25                    | 1020                    | 3              | 850              | 40                  | 76.74              |
| 12          | 25                    | 1080                    | 4              | 800              | 35                  | 91.22              |
| 13          | 30                    | 900                     | 6              | 850              | 35                  | 61.54              |
| 14          | 30                    | 960                     | 5              | 800              | 40                  | 62.47              |
| 15          | 30                    | 1020                    | 4              | 950              | 25                  | 68.78              |
| 16          | 30                    | 1080                    | 3              | 900              | 30                  | 72.46              |

3.2. Neural network training

To construct the GA-BP neural network model [8], we must first determine the input and output parameters. According to the principles to be followed in the parameter selection, combined with the prediction model whose output is the thickness of the infiltration layer, the influencing factors determined in this paper are: electrode spacing, holding temperature, holding time, source voltage, and working pressure. The 5-5-1 neural network model is selected, the network fitting training accuracy is 0.0001, the number of training samples is 2000, and the weights between nodes are optimized and estimated by genetic algorithm. The genetic algorithm selects the population as 50 and the algebra as 80. After network training, the fitness of the genetic algorithm is 2.5, and the neural network is much smaller than the required fitting error in 13 training samples, (MSE) is 8.4456e-006, indicating that the training samples are very representative that obtained from the input orthogonal experiment.

4. Optimized design and experimental verification

As shown in Fig. 2, a global simulation experiment is performed by using the trained BPNN. If you set the optimal target of 90μm or more, you can see that there are many optimized combinations, and the results are all greater than the maximum thickness value obtained by the orthogonal experiment. This paper extracts 7 optimized combinations, and selects two other combinations of prediction results to carry out verification experiments.
As shown in Fig.3, the trained BPNN is used to predict the setting level of each parameter, where each influence is averaged over time, and each parameter changes under 4 different fixed combinations of other parameters. It can be seen that the corresponding voltage, temperature and work can be considered to have a linear influence on the infiltration thickness rate based on certain assumptions. However, there are obviously different changes in the influence of the pole distance, and it is very sensitive to the combination of other parameters. This process shows that if you explore a better parameter combination, the optimal combination is probably not unique.
Table 2 shows the results of BP network prediction of permeable layer thickness and actual permeable layer thickness. Fig.4 is a cross-sectional view of the experimental sample. According to the data, the best process parameters are: the distance between electrodes is 15mm, the holding temperature is 1080°C, the holding time is 4.5h, the source voltage is 950V, the working pressure is 25Pa, the actual layer thickness is 95.0μm, and the predicted layer thickness is 97.5μm.

Fig.4 Photographs of tissues of different samples

Fig.5 shows the comparison between the predicted value of the seepage layer thickness and the real value, and the prediction and evaluation results of the neural network model. The analysis results show that the maximum error between the randomly selected simulation results and the experimental results is only 3.6%, the mean square error (MSE) is 5.349, the average absolute error (MAE) is 2.314, and the absolute coefficient (R²) is 0.964. The neural network model is basically consistent with the results of the process parameter mapping and the experimental results, which is effective and reliable. With the combination of process parameters within the value range, the model can be used to predict the experimental results [9].

| Test Number | Electrode Distance/m m | Holding Temperature/℃ | Holding Time /h | Source Voltage/ V | Working Pressure/P a | Thickness Layer Predictive value/μm | Thickness Layer actual measuring/μm |
|-------------|------------------------|------------------------|-----------------|-------------------|----------------------|------------------------------------|-----------------------------------|
| 1           | 15                     | 1080                   | 4.5             | 950               | 25                   | 95.2                               | 93.1                              |
| 2           | 15                     | 1080                   | 6               | 950               | 25                   | 97.5                               | 95.0                              |
| 3           | 25                     | 1080                   | 5.5             | 800               | 33                   | 93.8                               | 91.2                              |
| 4           | 25                     | 1080                   | 5.5             | 830               | 40                   | 94.5                               | 92.3                              |
| 5           | 30                     | 1080                   | 6               | 900               | 40                   | 90.7                               | 88.2                              |
| 6           | 27                     | 960                    | 4               | 950               | 25                   | 60.5                               | 58.4                              |
| 7           | 30                     | 1080                   | 5               | 900               | 25                   | 77.8                               | 75.6                              |
Fig.5 (a) Comparison between the predicted value of the seepage layer thickness and the real value (b) The prediction and evaluation results of the neural network model

5. Conclusions
Aiming at the thickness of Shuanghui ion molybdenizing process infiltration layer, the GA-BPNN model was established to complete the optimization design of Shuanghui ion molybdenizing process parameters. The optimized prediction results are consistent with the actual measurement results, indicating that the forecast method is feasible which is based on BP neural network. The exploration results also show that, in combination with the selection of process parameters and optimization goals, the optimal combination of infiltration parameters is not unique. These results are very conducive to the selection of process parameters and are closer to actual production requirements. In addition, experimental verification shows that no matter to predict the optimal or various infiltration thicknesses, the recommended optimization prediction methods can obtain representative results. This article predicts the technological parameters of double glow ion molybdenum infiltration, which provides a good reference method for the optimization of the thickness of the double glow ion molybdenum infiltration in engineering practice.

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