BP Neural Network Simulation Model of Specific Capacity Decay Rate between Porous Carbon/Sulfur Composites and Batteries

Ma Jishou

***Abstract*— The decay rate of cell specific capacity is closely related to the physical structure parameters and test conditions of porous carbon materials. In this paper, BP neural network principle is used to establish the relationship model between them. The first 201 groups of 211 groups of effective data are used as training data, and the last 10 groups are used as prediction data. The average relative error of prediction is 16.28%. It provides a theoretical basis for the design of porous carbon anode materials.**

***Index Terms*— BP neural network; Porous carbon/sulfur materials; Specific capacity decay rate**

I. INTRODUCTION

In recent years exploration has made great progress in the field of lithium sulfur batteries, among them with carbon materials as the carrier of sulfur/carbon anode materials design and development of research, research in the field of current lithium sulfur batteries is very broad, because it has strong electronic conductivity and large specific surface area, high chemical stability, etc. Is a very ideal sulfonium mass storage materials[1]. However, at present, there are still many problems in lithium sulfur battery itself, and there is still a long way to replace lithium ion battery commercially. Researchers in related fields are constantly trying to study related problems.

Nazar et al[3] prepared spherical ordered mesoporous material (OMC), with a high surface area of 2445 m^2g^{-1} and a large pore capacity of 2.32cmg^{-1} fused with 70$wt\%$ sulfur, the positive electrode of S/OMC still showed excellent electrochemical performance. At the current density of 1C, the capacity remained 700mAhg^{-1} after the first discharge of 1070$mAhg^{-1}$,100 turns. Zhijie Gong[4] selected three kinds of carbon materials with different pore structure types, analyzed and compared the influences of different pore structures on sulfur/carbon materials, and concluded that carbon materials with more micropores and large pores are more suitable as carriers of sulfur, and carbon/sulfur composite anode materials prepared have better performance. Nanping Deng[5] explored the correlation between physical structure parameters of porous carbon in anode materials, test conditions and electrochemical properties of cells by using the correlation principle, which provided some guidance for exploring mathematical models of structure, test conditions and electrochemical properties of anode materials. It is important to analyze the physical structure and test conditions of porous carbon for exploring the electrochemical properties of the cell. BP neural network can process the information provided by the external environment through self-regulation, and can self-learn and organize the output value to keep approaching the expected value [6], which has a strong pattern recognition and prediction function. Using BP neural network to explore the relationship between each other is of great significance.

In this paper, 220 groups of experimental data were analyzed, and 211 groups of valid data were selected through data preprocessing. Then, BP neural network was used to establish the relationship model of pore distribution and size, carrying capacity, specific surface area, pore volume, battery test conditions and specific capacity decay rate of porous carbon materials. The first 201 groups of data were used as training data and the last 10 groups as prediction data to test the fitting effect of the model. It provides a theoretical basis for the design of porous carbon anode materials.

II. ESTABLISHMENT OF BP NEURAL NETWORK MODEL

In this paper, BP neural network is mainly used to establish relevant mathematical models. The attenuation rate of specific capacity of the battery is selected as the dependent variable, denoting as y. Eight factors that have significant influence on it are independent variables. The hypothesis is as follows: the percentage of micropores, mesoporous pores and macropores in the porous carbon material in the whole porous carbon material: the micropores are denoted as x_1; The mesopore is denoted as x_2; The big hole is x_3; The sulfur content is denoted as x_4; The specific surface area is x_5; The pore volume is denoted as x_6; And the test conditions of the assembled battery: the test multiplier is denoted as x_7 and the number of cycles x_8.

2.1 experimental data preprocessing

Firstly, data were processed in this paper. In order to facilitate the calculation, the percentages of microporous x1, mesoporous x2, macroporous x3 and sulfur content x4 are converted into Numbers. Such as: 20%, 60% directly into: 20,60. The outliers were eliminated and 211 groups of valid data were finally selected for research and analysis. Partial data are shown in the following table:

Manuscript received July 23, 201

Ma Jishou, Tianjin polytechnic university School of mathematical sciences,Tianjin, 300387

Table 1 relevant experimental data

serial number	microporous	mesoporous	big hole	Sulfur loads	Specific Surface area	Pore volume	Test rate	number of cycles	Specific capacity Decay rate
1	100	0	0	53.4	1231	0.91	0.5	200	0.34
2	100	0	0	52.5	1133	0.86	0.5	200	0.34
3	100	0	0	50.3	991	0.82	0.5	200	0.38
4	100	0	0	50	1438	1.12	0.5	200	0.34
5	0	100	0	60	3164	1.88	0.5	800	0.06
					... ...				
210	0	100	0	57.4	1036	0.806	0.5	300	0.17
211	20	80	0	72	1013	1.26	0.5	200	0.1

2.2 Model establishment and experimental data prediction

2.2.1 BP neural network modeling

BP neural network is a multi-layer feedforward neural network, which consists of output layer, hidden layer and output layer. Neurons in the hidden layer can have multiple layers, and each layer only affects the next layer [7]. The network has the characteristics of signal forward transmission and error back propagation.

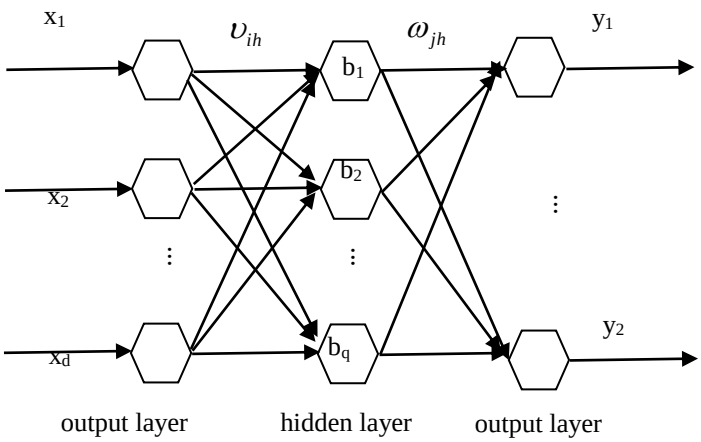

Figure 1 BP neural network simulation diagram

As shown in the figure above: X is the input value, Y is the predicted value, υ and ω is the weight value of the neural network. Before BP neural network prediction, the network needs to be trained first, so that it has associative memory and prediction ability [8].

The specific steps are as follows:

Step1. Initialization weight $\upsilon_{ik}, \omega_{hj}$;

Step2. Calculate the input received by the *h* th neuron in the hidden layer

$\alpha_h = \sum_{i=1}^{d} v_{ih} x_j$,b_h from the activation function *f*;

Step3.The input received by the jth neuron in the output layer is calculated as

$$\beta_j = \sum_{h=1}^{q} \omega_{hj} b_h$$

Step4. Calculate the actual output $\hat{y}_k = (\hat{y}_1^k, \hat{y}_2^k, \cdots \hat{y}_l^k)$,Among them $\hat{y}_j^k = f(\beta_j - \theta_j)$;

Step5. Calculate error function $E_k = \frac{1}{2}\sum_{j=1}^{l}(\hat{y}_j^k - y_j^k)^2$;

Step6. Adjust the link weight of hidden layer and output layer: $\Delta\omega_{hj} = \eta\hat{y}_j^k(1-\hat{y}_j^k)(y_j^k - \hat{y}_j^k)b_k$;

Step7. Adjust the threshold of the output layer: $\Delta\theta_j = -\eta\hat{y}_j^k(1-\hat{y}_j^k)(\hat{y}_j - \hat{y}_j^k)$;

Step8. Adjust the link weight of input layer and hidden layer:

$$\Delta\upsilon_{ih} = \eta b_h(1-b_h)\sum_{j=1}^{l}\omega_{hj}\hat{y}_j^k(1-\hat{y}_j^k)(y_j^k - \hat{y}_j^k)x_i$$

Step9. Adjust the threshold of hidden layer:

$$\Delta\theta_j = -\eta b_h(1-b_h)\sum_{j=1}^{l}\omega_{hj}\hat{y}_j^k(1-\hat{y}_j^k)(y_j^k - \hat{y}_j^k)$$

;

Step10. Repeat steps 2-9, Stop when E_k is small enough.

2.2.2 prediction of experimental data

In this paper, 211 groups of experimental data are put into BP neural network model for simulation test. The prediction results of the last 10 groups of data in table 2 are shown in the following table:

Table 2 actual and predicted specific capacity attenuation rates

serial number	The attenuation rate of actual battery specific capacity	BP neural network predicts the attenuation rate of specific capacity
1	0.7	0.664
2	0.45	0.521
3	0.67	0.723
4	1.15	1.481
5	0.98	0.804
6	1.47	1.145
7	1.36	1.069
8	1.21	0.834
9	0.17	0.155
10	0.1	0.104

It can be concluded from table 2 that the group with the largest relative error is group 8, the actual value is 1.21, the predicted value is 0.834, and the relative error rate is 31.09%. The group with the smallest relative error was the 10th group, with the actual value of 0.1, the predicted value of 0.104, and the relative error rate of 3.59%. The average relative error rate was 16.28%, and the fitting effect was good.

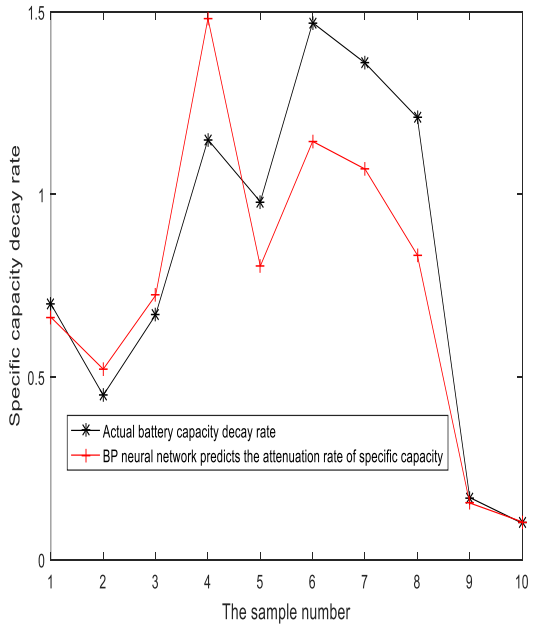

Fig.2 comparison of attenuation rate of specific capacity of BP neural network batteries

ENDNOTES

BP neural network model was used to explore the relationship between the decay rate of specific capacity of the battery and the physical structure parameters and test conditions of porous carbon. Good prediction results were obtained, with an average relative error rate of 16.28%. It is shown that BP network can well fit the relationship between dependent variables and independent variables, and this model will provide certain theoretical guidance for the design of physical structure parameters and test conditions of porous carbon.

REFERENCE

[1]A. Manthiram, Y. Z. Fu, Y. S. Su. Challeges and prospects of lithium–sulfur [J]. Acc. Chem. Res., 2013, 46, 1125–1134.

[2]Li xiang. Preparation and electrochemical properties of lithium sulfur battery sulfur/biomass carbon and nanometer lithium sulfide/porous carbon composite anode materials [D]. Zhejiang university,2017.

[3]He Guang, Jii Xiulei, Nazar Linda. High “C”rate Li-S cathodes:sulfur imbibed bimodal porous carbons [J].Energy&Envronmental Science,2011, 4(8):2878-2883.

[4]Zhijie Gong. Preparation and electrochemical properties of sulfur/porous carbon composite anode materials[D].Zhejiang university,2016.

[5]Nanping Deng. Preparation and properties of honeycomb porous carbon nanofiber anode material and aramane membrane for lithium sulfur battery[D].Tianjin polytechnic university,2018.

[6]Biaocan Ling , Jiabin Yang. Comparison of BP and RBF neural network in fault diagnosis of motor rolling bearing[J].Journal of north China institute of science and technology,2018,15(06):53 -57.

[7]Kangwei Fu, Xueqiang Zhang, Peng yan. Application of BP neural network algorithm in prediction of gas hydrate accumulation in continental area[J].Geophysical and geochemical exploration,2019,43(03):486-493.

[8]MATLAB Chinese BBS. MATLAB neural network 30 case analysis[M].Beijing: Beijing university of aeronautics and astronautics press,2010,73-76, 2-44.