Z. X. LI, Z. P. LIU, J. T. YU

ISSN 0543-5846
METABK 64(1-2) 72-74 (2025)
UDC: 678.7:661.183.2:539.32:620.17=111

PREDICTION OF CARBON BLACK/CARBON NANOTUBE REINFORCED POLYDIMETHYLSILOXANE PROPERTIES BASED ON BP NEURAL NETWORK

Received – Primljeno: 2024-04-19
Accepted – Prihvaćeno: 2024-07-19
Original Scientific Paper – Izvorni znanstveni rad

Sensory structure integration is the future development trend of flexible robots. At present, polydimethylsiloxane (PDMS) is often used as the main structural material for flexible robots, in which the addition of conductive fillers can achieve the perception of external forces and temperature. Therefore, it is of great research value to explore the road-writing properties of doped PDMS. This paper focuses on the mechanical properties of carbon black (CB)/carbon nanotubes (CNTs) doped PDMS on the line, aiming to promote the development of flexible robot industry.

Keywords: polydimethylsiloxane, carbon black, Young's modulus, tensile test, neural network

INTRODUCTION

Machine learning helps to accelerate the research and development process of composites, as well as understanding and optimising the properties and processes of polymer nanocomposites[1-3]. The use of machine learning to predict the properties of polymer nanocomposites based on their composition and structure is a promising approach in materials science. Doping has been shown to be effective in improving the mechanical and electrical properties of materials, so doping CBs and CNTs in PDMS can effectively improve the properties of composites to make them meet the demands of flexible robots.CBs and and CNTs belong to the carbon family of materials, which has a wide range of applications due to its excellent chemical, mechanical and electronic properties[4]. Training machine learning models from datasets can learn the relationship between composition, structure and properties of polymer nanocomposites. These datasets can include information on different combinations of polymers, nanomaterials and related properties. By using these data to train machine learning algorithms, different models can be developed that can accurately predict the properties of novel polymer nanocomposites. Therefore, in this paper, a study on the mechanical properties of PDMS composites doped with different concentrations of CB and CNTs has been carried out with the aim of enhancing the mechanical properties of composites for use in soft-bodied robots[5,6].

Materials and methods

CB model N110, CNTs length is about 10 μm, diameter is about 20 nm, PDMS is Dow Corning 184, all the above materials are purchased from Jingdong Mall.

Z. X. Li, Z. P. Liu, J. T. Yu, (E-mail: lizhanxian@nets.edu.cn) School of Mechanical Engineering North China University of Science and Technology, Tangshan, Hebei, China.

Experimental results and discussion

Firstly, take appropriate amount of agent A of PDMS and appropriate amount of CB and CNTs, mix them in a homogeneous mixer at 900 rpm for 3h, then add agent B of PDMS and mix them evenly for 10min. Afterwards, the prepared composites were poured into moulds to make standard parts, and the composites were mechanically tested using a universal testing machine. The relationship between the mechanical properties of the composites and the concentration of nanofillers is shown in Table 1.

From Figure 1, it can be seen that the Young's modulus of PDMS is about 750kPa, however, the Young's modulus increases by about 40,8% and 98,26% with the addition of 3wt.% CB and 4wt.% CNTs, respectively. From Figure 2, it can be seen that the tensile strength of the composites increased by about 32,13% and 30,57% after addition of 3wt.% CB and 4wt.% CNTs, respectively.

Table 1 **Relationship between mechanical properties of composites and nanofiller concentration**

Sample	wt.%CB	wt.%CNTs	Young's Modulus/ kPa	Tensile Strength/ MPa
1	0	0	750	4,22
2	1	0	774	4,43
3	2	0	834	4,87
4	3	0	1 056	5,84
5	4	0	953	5,51
6	0	1	845	4,59
7	0	2	980	4,91
8	0	3	1 375	5,36
9	0	4	1 487	6,23
10	1	1	893	4,87
11	1	2	1 194	5,49
12	1	3	1 409	6,81
13	1	1	824	4,89
14	2	1	994	5,87
15	3	1	1 206	6,32

It should be pointed out that the mechanical property enhancement of the composites is rather reduced when the concentration of CB is too high (wt.%), which may be due to the agglomeration of CB in PDMS when the concentration is too high. The results show that the Young's modulus and tensile strength of the composites filled with nano conductive fillers increased linearly in the range of nano filler concentrations with significant enhancement. Notably, at the same nanofiller loading, 1D CNTs showed the strongest system enhancement compared to CB. This may be due to the large specific surface area and aspect ratio of CNTs.

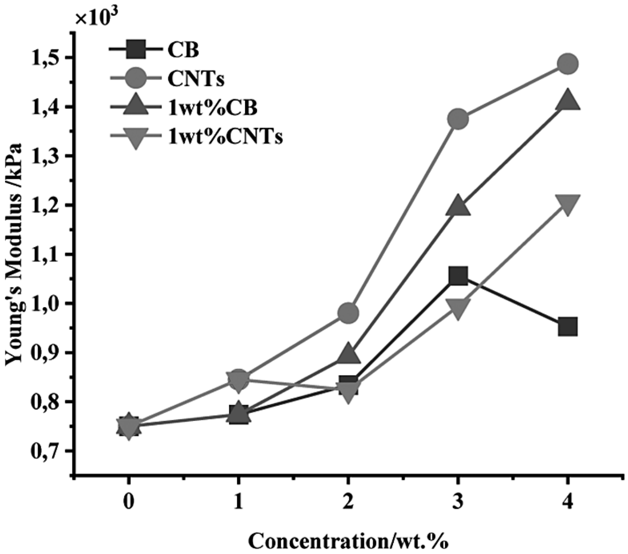

Figure 1 Young's modulus of composites at different concentrations

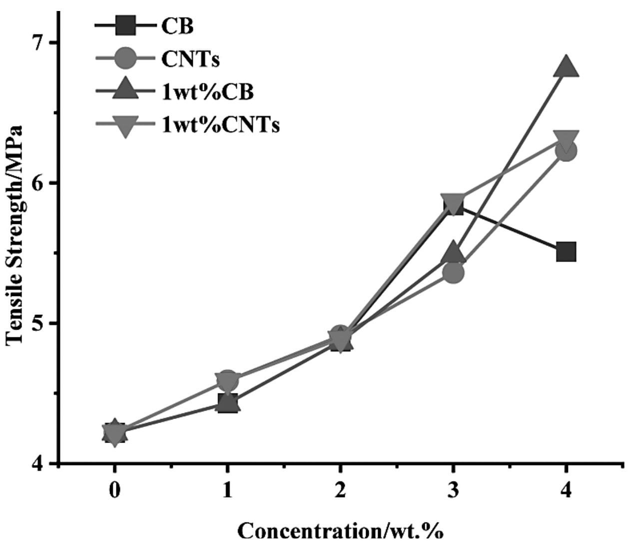

Figure 2 Tensile Strength of composites at different concentrations

BP neural network has arbitrarily complex pattern classification ability and excellent multi-dimensional function mapping ability, which solves the Exclusive or and some other problems that cannot be solved by simple perceptron. Structurally, BP network has input, hidden and output layers; essentially, the BP algorithm is to take the network error squared as the objective function, using the gradient descent method to calculate the minimum value of the objective function. Therefore, in this paper, BP neural network is used to predict the performance of composite materials.

In BP neural networks the number of hidden layers and the number of neurons have a crucial impact on the fitting results, so we firstly determined the optimal number of hidden layers and the number of neurons using R^2 as a parameter, see Figures 3~6.

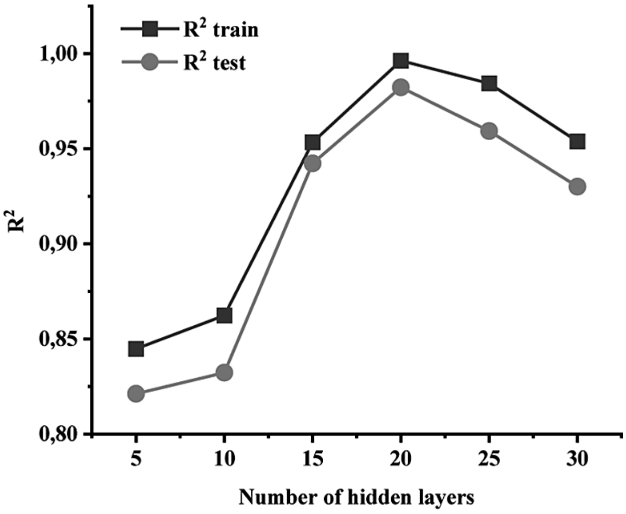

Figure 3 Neural network R^2 with different number of hidden layers for predicting Young's modulus

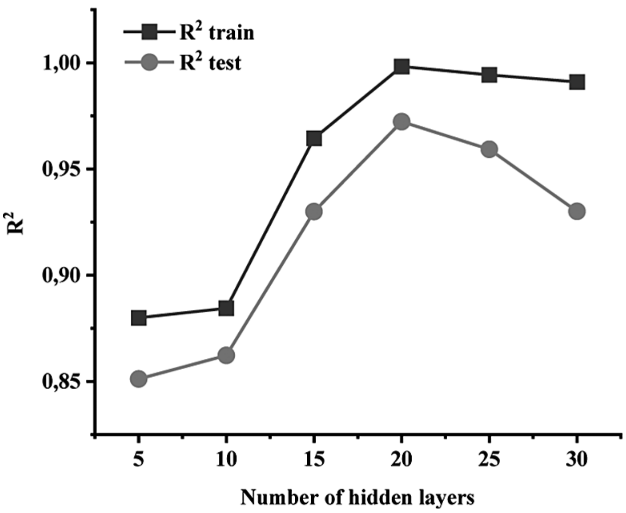

Figure 4 Neural network R^2 with different number of hidden layers for predicting tensile strength

From Figures 3~4 it can be seen that as the number of hidden layers increases the fitting effect first gets better and then decreases. The best prediction performance for Young's modulus and sum is obtained when the number of hidden layers is 20, and the prediction effect decreases when the number of hidden layers becomes more, which is caused by overfitting.

From Figures 5 to 6, it can be seen that when the number of hidden layers is 2, the fitting effect becomes better and then decreases with the increase of the number of neurons in each layer. The best prediction performance for Young's modulus and tensile strength is obtained when the number of neurons per layer is 15, and the prediction effect decreases when the number of neurons per layer becomes more, which is also caused by the occurrence of overfitting. Therefore, the optimal parameters of the BP neural network were determined to be 20 hidden layers with 15 neurons per layer.

The prediction results using the optimised BP neural network are shown in Table 2, where it can be seen that the optimised BP neural network has a high level of prediction of composite properties. The R^2 for Young's modulus prediction reaches 0,9853 and for tensile strength prediction reaches 0,9953, which shows the good prediction performance of the optimised BP neural network. In

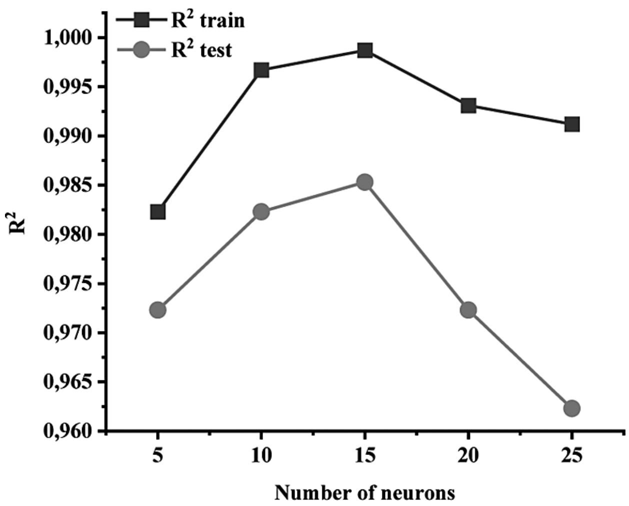

Figure 5 Neural network R^2 with different number of neurons for predicting Young's modulus

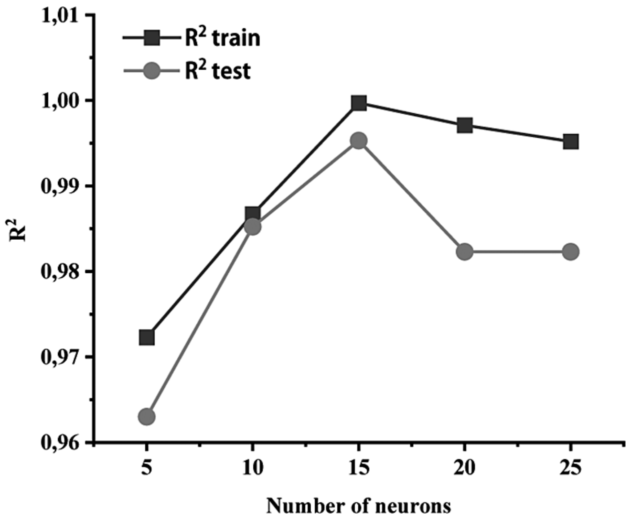

Figure 6 Neural network R^2 with different number of neurons for predicting tensile strength

Table 2 **Optimised BP neural network performance prediction results**

	R^2 train	R^2 test	MAE	MSE
Young's modulus	0,9987	0,9853	0,2316	0,1344
Tensile strength	0,9997	0,9953	0,1245	0,1534

where: MSE is the minimum squared error; MAE is the mean absolute error.

order to further assess the accuracy of the BP model implemented in this paper, MSE and MAE were also compared and the results are collected in Table 2. The MAE and MSE are widely recognised as an important validation criterion for ML models, where the lower the value, the more accurate the prediction of the desired performance. The MAE and MSE predicted for Young's modulus are 0,2316 and 0,1344, respectively, showing high prediction accuracy. The MAE and MSE predicted for tensile strength were 0,1245 and 0,1534, respectively, which also verified the accuracy of prediction.

CONCLUSION

In this paper, the effect of CB and CNTs doping on the mechanical properties of PDMS was analysed and the prediction of the properties of the composites was achieved using BP neural network. The Young's modulus and tensile strength of the doped composites were increased by 40,8% and 98,26%, respectively, compared to PDMS, which shows the great help of doping in improving the properties of composites. In this paper, the two most important parameters of the BP neural network, i.e., the number of hidden layers and the number of neurons per layer, are optimised. The optimised number of hidden layers is 20 and the number of neurons per layer is 15.The optimised BP neural network demonstrates good performance in predicting Young's modulus and tensile strength of composites. The prediction accuracy of 0,9853 for Young's modulus and 0,9953 for tensile strength shows the strong performance of the optimised BP neural network..

REFERENCES

[1] Song L., Wang D., Liu X., et al. Prediction of mechanical properties of composite materials using multimodal fusion learning[J]. Sensors and Actuators, A. Physical, 2023:358.

[2] Feng Z., Ma Q., An Z., et al. New Fatigue Life Prediction Model for Composite Materials Considering Load Interaction Effects[J].International Journal of Applied Mechanics, 2023, 15(09). DOI:10.1142/S175882512350076X.

[3] Yuan R., Chen R., Li H., et al. Dynamic Reliability Evaluation and Life Prediction of Transmission System of Multi-Performance Degraded Wind Turbine[J]. Computer modelling in engineering and science, 2023(6):17. DOI:10.32604/cmes.2023.023788.

[4] Vernooij J. E. M., Koning N. J., Geurts J. W., et al. Performance and usability of pre-operative prediction models for 30-day peri-operative mortality risk: a systematic review[J]. Anaesthesia: Journal of the Association of Anaesthetists of Great Britain and Ireland, 2023.DOI:10.1111/anae.15988.

[5] Lyu J., Mei H., Zu L., et al. Modeling Method of C/C-ZrC Composites and Prediction of Equivalent Thermal Conductivity Tensor Based on Asymptotic Homogenization[J]. Computer modelling in engineering and science, 2024, 138(1): 391-410. DOI:10.32604/cmes.2023.030614.

[6] Ning H , Chen F , Yunfeng S U ,et al.Modeling and prediction of tribological properties of copper/aluminum-graphite self-lubricating composites using machine learning algorithms[J]. Friction, 2024, 12(6): 1322-1340. DOI: 10.1007/s40544-023-0847-2.

Note: The responsible translator for English language is Z. P. Liu - North China University of Science and Technology