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Research of dielectric properties of carbon nanotubes and their composites using the method of artificial intelligence

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This article discusses the development of an expert system based on an artificial neural network for analyzing the dielectric properties of single-layer carbon nanotubes. By measuring and analyzing the single-walled carbon nanotube/polyurethane composites, multi-walled carbon nanotube/silicone rubber conductive polymer materials, and single-walled carbon nanotube/epoxy resin composite materials we can get the specific numerical dielectric characteristics which can reduce the workload of the researchers, reduce research cost and shorten the time and improve efficiency.

Keywords: carbon nanotubes, artificial neural network, expert system, dielectric properties.

Рассматривается экспертная система на основе искусственной нейронной сети для анализа диэлектрических свойств однослойных углеродных нанотрубок. Измеряя и анализируя однослойные углеродные нанотрубки (полиуретановые композиты, многостенные углеродные нанотрубки), проводящие полимерные материалы из силиконовой резины, одностенные композитные материалы из углеродных нанотрубок/эпоксидных смол, можно получить конкретные численные диэлектрические характеристики, которые могут снизить загруженность исследователей и снизить затраты на исследования.

Дослідження діелектричних властивостей вуглецевих нанотрубок і їх композитів методом штучного інтелекту. *Y.Zeng, X.Guo*.

Розглядається розробка експертної системи на основі штучної нейронної мережі для аналізу діелектричних властивостей одношарових вуглецевих нанотрубок. Вимірюючи і аналізуючи одношарові вуглецеві нанотрубки (поліуретанові композити, багатостінні вуглецеві нанотрубки), які проводять полімерні матеріали із силіконової гуми, одностінні композитні матеріали з вуглецевих нанотрубок епоксидних смол, ми можемо отримати конкретні чисельні діелектричні характеристики, які можуть знизити завантаженість дослідників і знизити витрати на дослідження.

1. Introduction

Carbon nanotubes (CNTs) are hollow tubes made of sheets of graphene formed from carbon atoms. These have high aspect ratio, excellent elongation, flexibility, elastic modulus, strong acid and alkali resistance and thermal properties [1]. For a long time, material researchers needed to carry out a large number of experiments through permanent adjustment of experimental parameters, and then according to the performance of the selection, finally they chose one or several parameters which can meet the requirements of the material composition. This research method consumes a lot of manpower, material resources and time, and it is characterized by great contingency and blindness [2].

With the continuous development of computer science and artificial intelligence, artificial neural network technology research methods appeared. Their structure is built by simulating the structural characteristics of biological nerves and is similar to the information processing model formed by the interconnection of neurons in the brain. With self-learning, adaptive ability, good fault tolerance, a strong memory function, and a prediction function, it can quickly find the optimal solution [3]. Therefore, it is widely used in material design, optimization of preparation parameters and prediction of material properties. The artificial neural network has expanded people's understanding and ability to control the environment; this aroused great attention of researchers in various fields; the applications are expanding and new research continues to emerge. The combinations of the artificial neural network with other technologies allow one to apply them well in many fields and have a good development prospect [4].

Therefore, carbon nanotubes have great application prospects, and have been a research hotspot at home and abroad in recent years. B.Chen et al. discussed the common synthesis methods of carbon nanotubes, an arc discharge method, a vapor deposition method and a flame method in detail. Typical applications in sensors, supercapacitors, catalysis, hydrogen storage and medicine are summarized [5]. M.Varga et al. analyzed the research progress and application prospects of carbon nanotubes in the fields of photoelectric devices, supercapacitors and hydrogen storage materials [6]. X.Liu et al. summarized and commented the application of carbon nanotubes in many fields in recent years, and predicted several application prospects and development potential of carbon nanotubes, providing a reference for the further development and application of the carbon nanotubes [7]. In this paper, an artificial neural network expert system for carbon nanotube composites was established to sort, analyze and deal with the processing and sample properties of carbon nanotube composites. The artificial neural network expert system was used to reduce the workload of researchers, reduce the research cost, shorten the research time and improve the efficiency.

2. Research methods

2.1 Establishing artificial neural network and expert system

Artificial neural networks are good at numerical calculation and dealing with complex multivariate nonlinear problems. Expert systems are good at using knowledge and reasoning to solve problems. They both have advantages and disadvantages as shown in Table 1. The artificial neural network and expert system are combined together to solve the problem. They can learn from each other and strengthen each other.

The expert system of CNTs can be divided into a database management function, a neural network training function and a neural network prediction function. Its composition is shown in Fig. 1.

Table 1. Comparison between an artificial neural network and an expert system

Comparison of object	Expert system	Neural network
Knowledge acquisition	Mainly relies on transplanting the knowledge of domain experts into the system. Features: trouble, low efficiency	Learning directly from numerical examples or the traditional artificial intelligence technology has been acquired by the knowledge of special cases into the neural network distributed storage [8]. Features: time-saving and high efficiency
Application field	It can only be used in a fairly narrow field of expertise. Features: narrow application range	You can solve problems in any field (as long as you have samples). Features: wide application range
Reasoning ability	The reasoning method is simple, the control strategy is not flexible and the reasoning efficiency is low. Features: low reasoning ability	It has strong nonlinear fitting ability and can map any complex nonlinear relationship. Features: high reasoning ability
Intelligent level	Without self-learning ability and associative memory function they cannot improve, develop and innovate the knowledge in the process of operation [9]. Features: low intelligence level, no self-learning and associative memory function	Sample input is used for learning and training, and the learning algorithm is diversified; this imitates human brain thinking and can be inferred by associative memory, recognition and analogy [10]. Features: high level of intelligence, self-learning and associative memory function

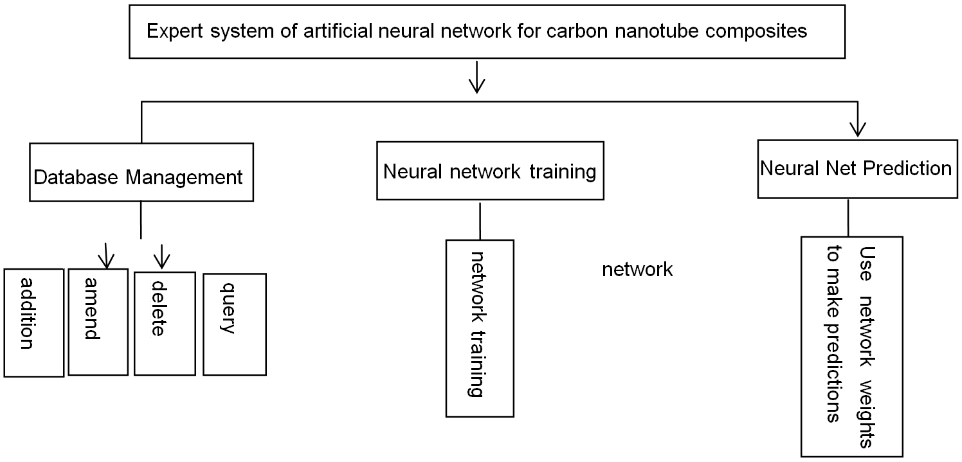

Fig. 1. System module organization diagram.

Software Development Environment (SDE) is also known as integrated project support environment. Writing and operation needs the support of computer software; a computer language is the basis of the software implementation. Now, with the development of computer technology, computer hardware and software of the operating system has been updated, including C# as an object-oriented programming language, it is widely used due to its powerful functions, simplicity and flexibility.

The operating system used in this paper is Windows7; the tool environment used for writing is Microsoft Visual Studio; and the data management is Microsoft SQL Server database. The development and design of the artificial neural network expert system based on the BP neural network is realized. ADO.NET is used to access and operate data sources. The general steps for ADO.NET to access data sources are as follows:

– Create a connection to the data source;

– Find the required Data record Set and cache the record Set into the Data Set;

– If more than one data is needed, return to step 2 to continue adding;

– After adding data successfully, close the data connection;

– Use the Data Set to perform the required Data access operations.

2.2 Database management

Database management is the basis of the whole artificial neural network expert system, and the stored human expert data should be as rich and accurate as possible. As shown in Fig. 1, the management and maintenance of the database is divided into adding and modifying, deleting and performance of query.

(1) Add: add the latest human expert data according to the type of expert data, add to the corresponding material Table. The flow of the add operation is shown in Fig. 2.

– Modification: modify the expert data in the man-machine interface of the corresponding materials to update the expert data of the system.

– Delete: delete the wrong expert data in the expert system.

– Query: after the establishment of the human expert database, there will be new expert data added to the database, which will lead to very large amount of data in the database. It is very difficult to find the required data, then the user can use the data query function.

2.3 Neural network training and prediction

During the material processing, there are many variables that affect the final performance, and the relationship between them is very complex. However, we use an artificial neural network to predict the performance of materials based on the existing data, which provides a certain reference value for researchers. In this paper, a BP neural network with an additional momentum factor and a learning rate variable is used to train expert data. After training, the network connection weight matrix obtained by the BP neural network can be used to predict relevant material data by the artificial neural network. The process is shown in Fig. 3.

2.4 The realization of the BP neural network

The standard BP neural network model has some defects, such as slow learning rate and convergence speed, and the local mini-

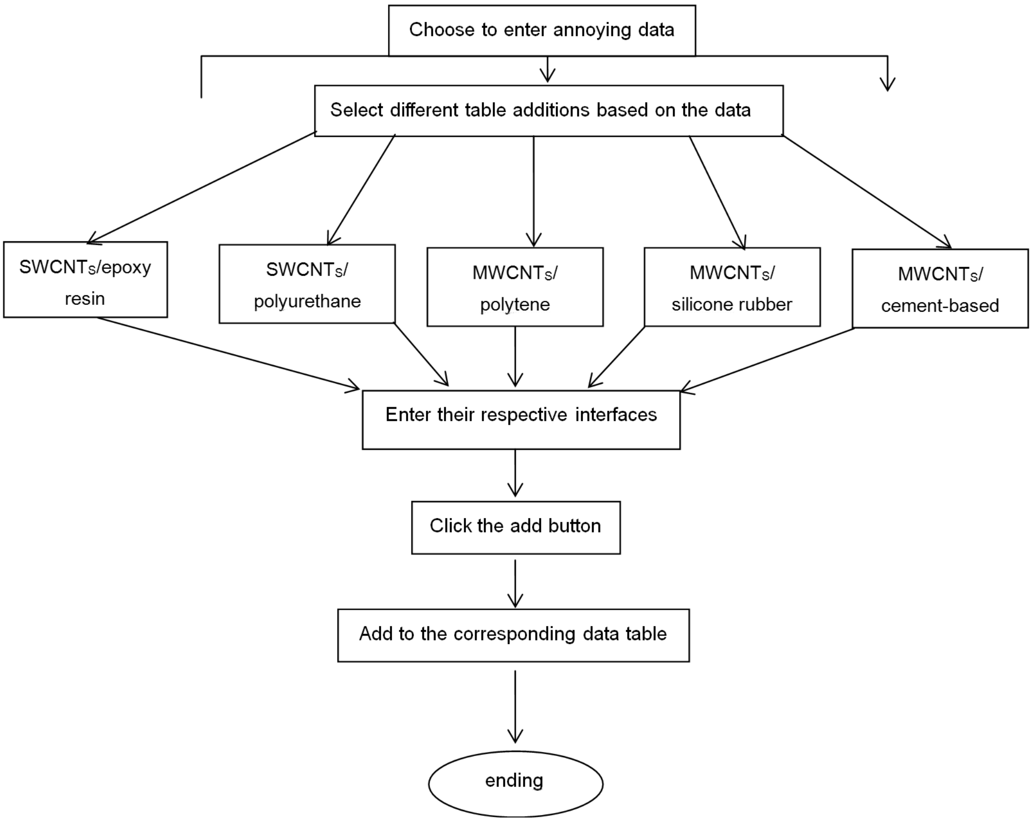

Fig. 2. Flow chart of data addition.

mum rather than the global minimum may be obtained during the network training. Therefore, the improved BP neural network is adopted to increase the performance of the BP neural network to some extent by adding the momentum factor and learning rate variable. The improved BP neural network uses η to represent the learning rate and α for the momentum factor, then the adjustment of the connection weight matrix of the output layer is:

$$\Delta M_{jk}(t) = \eta(1-\alpha)\frac{\partial E}{\partial M_{jk}(t-1)} + \alpha\Delta M_{jk}(t-1). \quad (1)$$

The adjustment of the connection weight matrix of the hidden layer is:

$$\Delta W_{ij}(t) = \eta(1-\alpha)\frac{\partial E}{\partial W_{ij}(t-1)} + \alpha\Delta W_{ij}(t-1). \quad (2)$$

The adjusted connection weight matrix is:

$$W_{ij}(t) = W_{ij}(t-1) + \Delta W_{ij}(t) = W_{ij}(t-1) + \eta(1-\alpha)\frac{\partial E}{\partial W_{ij}(t-1)} + \alpha\Delta W_{ij}(t-1). \quad (3)$$

$$M_{jk}(t) = M_{ij}(t-1) + \Delta M_{ij}(t) = M_{ij}(t-1) + \eta(1-\alpha)\frac{\partial E}{\partial M_{ij}(t-1)} + \alpha\Delta M_{ij}(t-1). \quad (4)$$

Among then, $M_{jk}(t)$ and $W_{ij}(t)$ are respectively the connection weight matrix of the output layer and the hidden layer after adjusting t times; $\Delta M_{jk}(t-1)$ and $\Delta W_{ij}(t-1)$ are corrections of the connection weight after adjustment $(t-1)$. The improved BP neural network needs to select an appropriate learning rate. If the learning rate is too large, the algorithm may oscillate and cause instability. If the learning rate is too small, the convergence speed will be slow. With addition of the momentum factor, the network training can provide the next correction affecting the previous one to reduce the oscillation and avoid falling into the local minimum.

In the network training with this expert system, only one hidden layer is usually selected, and two or more layers can be selected as required. The number of neuron nodes in the hidden layer is calculated according to the empirical formula $h = \sqrt{n \cdot m} + a$; so as to calculate the number of neuron nodes in the hidden layer h, as the initial value of network regulation, the

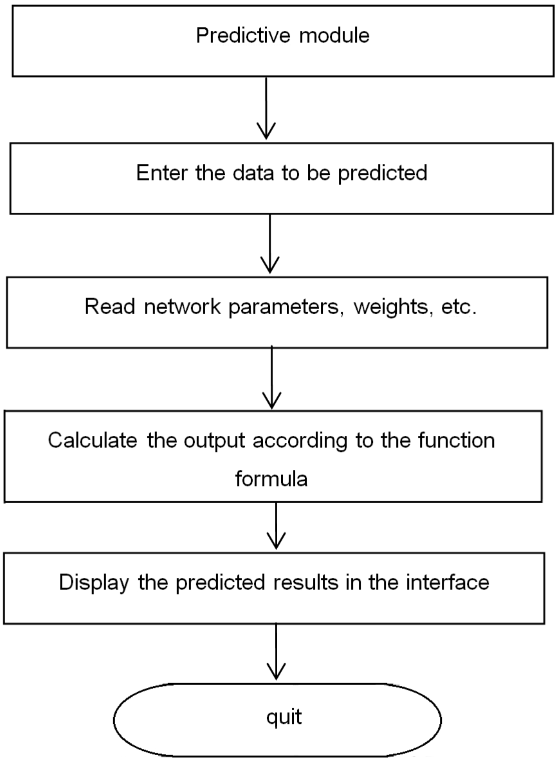

Fig. 3. Flow chart of BP neural network prediction.

process of the network training using the improved BP neural network is as follows:

– Set the training frequency (denoted by N), the training accuracy (denoted by E), the learning rate is η, the momentum item of the BP neural network is α, and make $N(0,\infty)$, $E\in(0,1)$ $\eta\in(0.01,1)$, $\alpha\in(0,1)$.

– The connection weight matrix is initialized to generate a new neural network.

– Enter a set of trained expert data in the order stored in the database.

– The error of the network output is calculated, the back propagation of the error signal is carried out, and the connection weight is corrected.

– The next material data sample is trained with the corrected connection weight, and then the last expert data sample is alternately trained to calculate the total average error of the network training. If the total average error is less than the preset precision E, the training is successful and ends, and the connection weight matrix of expert data is saved at the same time. If the total average error is greater than the preset error E, go to step 6.

3. Results and discussion

3.1 Dielectric properties of single-walled carbon nanotubes/polyurethane carbon nanotubes composites

In the network training, the hidden layer is set as 2 layers, and the number of hidden layer nodes in the first layer and the second layer is set as 4 and 6 respectively; the training error is <0.08; the training frequency is less than 20,000 times; the learning rate is 0.4 and the momentum factor is 0.6. As shown in Table 2 and Fig. 4, the dielectric constant of single-walled carbon nanotubes/polyurethane composites is predicted to be stable at 8.5–12 GHz when the content of carbon nanotubes is 20 % according to the results of the network training. The real part of the dielectric constant ε_1 is approximately 33.48 ~ 34.45, and the imaginary part of the dielectric constant ε_2 is approximately 23.46 ~ 24.35.

3.2 Electromagnetic shielding effectiveness of multiwalled carbon nanotubes/silicon rubber conducting polymers

In the network training, the hidden layer is set as 1 layer, the number of nodes in the hidden layer is set as 4, the training error is less than 0.05, the training times are less than 20,000, the learning rate is 0.6, and the momentum factor is 0.6. As shown in Fig. 5, according to the results of the network training, the electromagnetic shielding efficiency of the multi-walled carbon nanotubes/silicon rubber conductive polymer material increases to approximately 24.82–26.68 dB with the increase of frequency to 100 ~ 1000 MHz when the content of carbon nanotubes is 8 %.

3.3 Dielectric properties of single-walled carbon nanotubes/epoxy resin composites

In the network training, the hidden layer is set as 1 layer, the number of hidden layer nodes is set as 4, the training error is less than the training times is less than

Table 2. Predicted values of dielectric constants of SWCNTs/polyurethane composites

Dielectric constant frequency, GHz	8	8.5	9	9.5	10	10.5	11	11.5	12	12.5
Real part	33.91	34.12	34.45	34.16	33.89	33.86	33.75	33.64	33.56	33.48
Imaginary part	23.46	23.56	24.35	24.29	24.16	23.89	23.95	23.78	23.72	23.65

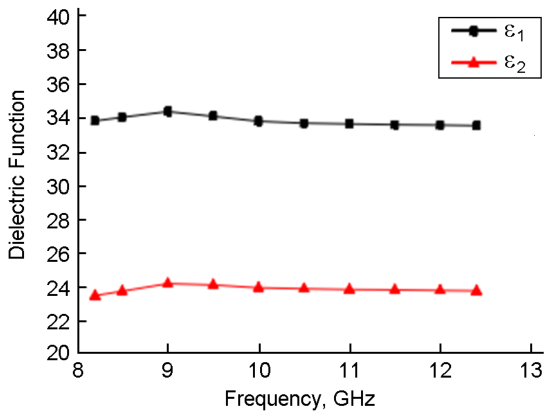

Fig. 4. Predicted values of dielectric constants of SWCNTs/polyurethane composites.

20,000 times, the learning rate is 0.6, and the momentum factor is 0.4. As shown in Table 3 and Fig. 6, the dielectric constant of SWCNTs/epoxy resin composites was predicted to be stable at 8.5–12 GHz; when the carbon nanotube content was 15 %, the real part of the dielectric constant ε_1 was about 52.32–54.91, and the virtual part of the dielectric constant ε_2 was about 56.93–59.86.

4. Conclusions

In this paper, the artificial neural network and expert system are combined together. By using Microsoft Visual Studio, Microsoft SQL Server database and a BP neural network, the artificial neural network expert system of carbon nanotube composite materials is established to optimize the training module of the BP neural network. The momentum factor, learning rate, hidden layer number, hidden layer node number and training times can be adjusted to make the network training as optimal as possible and realize the prediction of the BP neural network.

According to the results of the network training, it is predicted that the dielectric constant of single-walled carbon nanotubes/polyurethane composites is stable at 8.5–12 GHz when the content of carbon nanotubes is 20 %, the real part of the dielectric constant is approximately 33.48–34.45, and the imaginary part of the dielectric constant is approximately 23.46–24.35. When the content of carbon nanotubes is 8 %, the

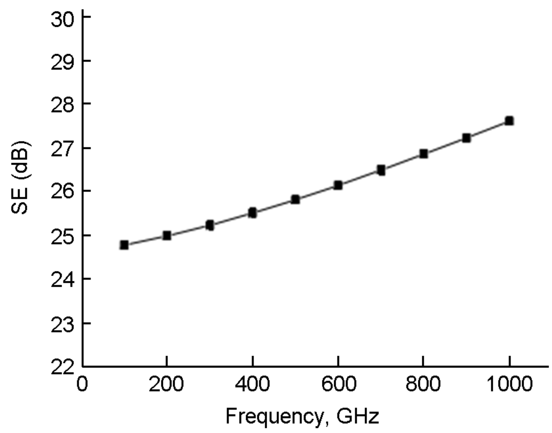

Fig. 5. Predicted value of electromagnetic shielding effectiveness of MWCNTs/ silicon rubber materials.

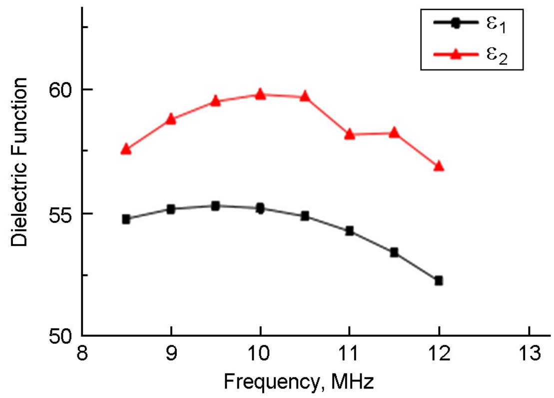

Fig. 6. Predicted values of dielectric constants of SWCNTs/epoxy resin composites.

electromagnetic shielding efficiency of multi-walled carbon nanotubes/silicon rubber conductive polymer materials is about 24.82–26.68 dB at 100 ~ 1000 MHz. When the content of carbon nanotubes was 15 %, the dielectric constant of the single-walled carbon nanotubes/epoxy resin composites ranged from 8.5 to 12 GHz. The real part of the dielectric constant ranged from 52.32 to 54.91, and the virtual part of the dielectric constant ranged from 56.93 to 59.86.

The artificial neural network expert system of carbon nanotube composites can achieve the expected functional goals and predict the properties of carbon nanotube

Table 3. Dielectric constants of SWCNTs/epoxy resin composites

Dielectric constant frequency, GHz	8.5	9	9.5	10	10.5	11	11.5	12
Real part	54.82	54.91	54.86	54.56	54.21	54.13	53.87	52.32
Virtual part	57.42	59.12	59.56	59.86	59.74	57.56	57.63	56.93

composites. The use of the artificial neural network expert system can effectively reduce the workload of researchers, reduce the research cost, shorten the research time and improve the research efficiency.

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