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Artificial Neural Network Based Prediction Hardness of Al2024-Multiwall Carbon Nanotube Composite Prepared by Mechanical Alloying

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ABSTRACT

In this study, artificial neural network was used to predict the microhardness of Al2024-multiwall carbon nanotube(MWCNT) composite prepared by mechanical alloying. Accordingly, the operational condition, i.e., the amount of reinforcement, ball to powder weight ratio, compaction pressure, milling time, time and temperature of sintering, as well as vial speed were selected as independent input and the mean micro-hardness of composites was selected as model output. To train the model, a Multilayer perceptron neural network structure and feed-forward back propagation algorithm has been employed. After testing many different ANN architectures, an optimal structure of the model i.e. 7-25-1 was obtained. The predicted results, with a correlation relation between 0.982 and 0.9952 and 3.26% mean absolute error, show a very good agreement with the experimental values. Furthermore, the ANN model was subjected to a sensitivity analysis and the significant inputs affecting hardness of the samples were determined.

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1. INTRODUCTION

Weight reduction of automobile and aircraft is one of the most important methods of improving the energy efficiency. Hence, a growing demand for application of metal matrix composites (MMCs) with higher strength to weight ratio was evolved. Due to high strength and stiffness of carbon nanotube (single wall and multi wall), they had excellent properties as strengthening agent for preparation of composites [1, 2]. Experimental results on multi-wall carbon nanotube (MWCNT) showed Young's modulus to be between 600 and 1100 GPa while the tensile strength ranged from 35 to 110 GPa [3]. These excellent mechanical properties combined with low density, i.e., 1.8 g/cm^3 make CNTs ideal candidate as reinforcement agent to prepare the high specific strength Nano-composites [4]. To the best of own knowledge, the main research efforts in the past decade have been done on the CNT reinforced polymer or ceramic matrix composites [5-7]. Some research were focused to manufacture the CNT/metal composites by different techniques such as sintering [8], hot extrusion [9, 10], spark plasma sintering [11-13], spark plasma extrusion [14], casting [15] and friction stir processing [16].

Mechanical alloying includes continuous impact, welding, fracturing and re-welding of powders through high energy ball milling of powder, e.g., planetary ball mill. In this method, the constituents would be effectively and homogeneously distributed within [17].

Artificial neural network (ANN) is a useful mathematical tool for materials research community [18-24]. ANN can solve relatively complex, nonlinear, multi-dimensional functional relationships after training by experience data. In this method, the transfer function between the elements plays a key role in quality of prediction. To the best of our knowledge, the multilayered perceptron (MLP) is the most common strategy in ANN [25]. In the present study, a MLP neural network was used for prediction of microhardness of Al2024-CNT composite, using reported data in literature as input.

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2. PRINCIPLE OF ARTIFICIAL NEURAL NETWORK

As illustrated in Figure 1, an ANN structure commonly is divided into three parts: input layer, hidden layer and output layer. The nodes or neurons, are connected by weighted inter-connections which resemble the intensity of the bioelectricity transferring among the nodes cells in an actual neural network. The trained results can be summarized in terms of weights and the biases [26].

The neurons numbers in the input and the output layer are fixed to be equal to that of input and output variables, whereas the hidden layer can include more than one layer, and in each layer the number of neurons is tolerant. Adjusting the structure of a network is a key role in improvement of performance network [27]. The structure of network can be expressed as:

$$N_{in} - \left[N_1 - N_2 - \cdots N_h\right]_h - N_{out} \tag{1}$$

where N_{in} and N_{out} refer to the number of input and output variables, respectively. Subscript h shows the number of hidden layers, while N_1, N_2 and N_h are the number of neurons in each hidden layer.

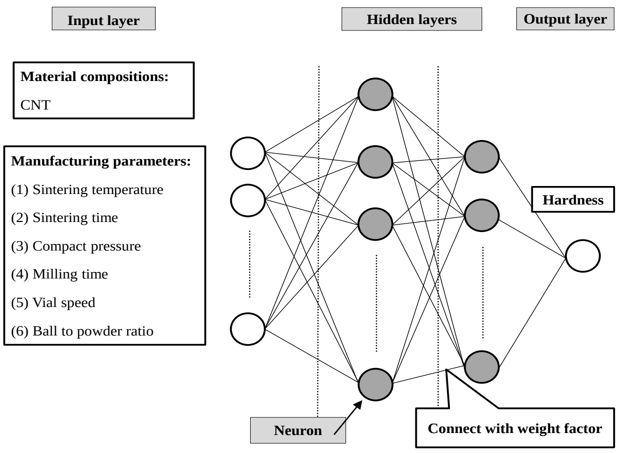

Figure 1. The schematic construction of an artificial neural network with input, output and testing parameters

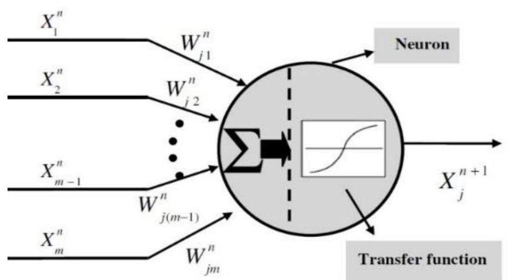

Figure 2. A schematic description of the relationship between the input and output vectors of one neuron

The network gets information from the input layer, analyses the data in the hidden layers, and then exports the results via the output layer. In each hidden layer and output layer, the neurons take the output of the neurons in the preceding layer as the input. The data are analyzed by transfer function with weights and bias in the neurons to obtain the output as shown in Figure 2, described by:

$$X_i^{(n)} = f\left(\sum_i w_{ji}^{(n)} x_i^{(n-1)} + b_j^{(n)}\right) \tag{2}$$

where $X_j^{(n)}$ is the output of node j in the nth layer, $W_{ji}^{(n)}$ the weight from node i in the $(n-1)$th layer to node j in the nth layer, and $b_j^{(n)}$ the bias of node j in the nth layer [28]. For ANN modeling commonly three transfer functions are used for the hidden and the output layers (Table 1).

Back-propagation (BP) algorithm is an iterative gradient descent approach, (i.e., one of the most widely used as training strategies for multi-layer networks) to minimize the mean squared error (MSE) between the predicted and desired values:

$$MSE = \frac{1}{2L}\sum_{T=1}^{L}\left[d(t)-p(t)\right]^2 \tag{3}$$

where L shows to the number of training patterns, d(t) is the desired output value, and p(t) the target output value predicted by the ANN for the tth pattern. During the training step, the network is represented with the data hundreds of cycles, the weights and biases are adapted until the suitable error level is obtained or the maximum iteration is achieved. This iterative adjustment of the weights and biases can be obtained as following:

$$w_{ji}^{(n)}(k) = w_{ji}^{(n)}(k-1) - \alpha\frac{\partial E}{\partial W_{ji}^{(n)}} \tag{4}$$

$$b_j^{(n)}(k) = b_j^{(n)}(k-1) - \alpha\frac{\partial E}{\partial b_j^{(n)}} \tag{5}$$

where α represents the learning rate, and k refers to the iteration [29].

TABLE 1. Transfer functions used in this study

Serial	Transfer function	Formula
1	Hyperbolic tangent sigmoid	$f(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$
2	Linear	$f(x) = x$
3	Log-sigmoid	$f(x) = \frac{1}{1+\exp(-x)}$

3. IMPLEMENTATION

Practically, an adequate amount of experimental data is necessary to develop a neural network with good performance. The architecture, transfer function, training strategy and other factors of the neural network should be carefully determined and changed through optimization. Thus, the well trained neural network can be applied to model the new input data in the same domain of the practical data base.

This procedure can be summarized as the following steps:

1. Collect and pre-procedure the practical data;
2. Train the ANN, and improve its configuration;
3. Evaluate the performance of the ANN, return to step 2 if the performance is not satisfactory;
4. Use the trained ANN for simulation or prediction.

The ANN programs were written in MATLAB software. A database containing 44 independent hardness experiments of Al2024-CNT composites performed under various conditions as well as different compositions gathered from the literature [8, 30-34], were used to train (35 groups of data) and test the ANN (9 groups of data). Material composition and manufacturing parameters were selected as the input parameters, and hardness was chosen as the output parameter (Table 2).

First, to increase the efficiency of the neural network, the experimental database was normalized. The applied normalizing process is represented by:

$$Xn = 0.8 \times \frac{X - X_{min}}{X_{max} - X_{min}} + 0.1 \tag{6}$$

where X_{max} and X_{min} are the maximum and minimum values of the independent variable X. Second, the experimental database was randomly divided into two parts. One part was used to train the network, and the other to test it. To facilitate the comparisons of performance for different network configurations, mean absolute percentage error (MAPE), sum of square errors (SSE) and root mean square error (RMSE) were introduced:

$$MAPE = \frac{1}{L}\left[\sum_{T=1}^{L} \frac{|d(t) - p(t)|}{d(t)}\right] \times 100 \tag{7}$$

$$SSE = \sum_{T=1}^{L} \left(d(t) - p(t)\right)^2 \tag{8}$$

$$RMSE = \sqrt{MSE} \tag{9}$$

TABLE 2. Input and output parameters of artificial neutral network

Input	
Material composition	Matrix (95-100 wt. %)
	CNT (0-5 wt. %)
Manufacturing parameters	Sintering temperature (ST) , i.e., 450-550 °C
	Sintering time (St) , i.e., 0.25-2 h
	Compact pressure (CP) , i.e., 41.36-1500 MPa
	Milling time (Mt) , i.e., 1-30 h
	Vial speed (VS), i.e., 300-350 rpm
	Ball to powder weight ratio (BPR) , i.e., 5-10
Output	
Mechanical property	Hardness (67.6-290.9 HV)

3. 1. Selection of ANN Architecture

Defining the architecture of the network can dramatically influence the performance of network. However, there is no distinct way to determine the hidden layer for a particular application [35]. In this case, a program has been presented to test various architectures of feed-forward back propagation ANN to determine the structure with the lowest mean absolute percentage error (MAPE) for the testing data set as depicts the flowchart in Figure 3. The program was run to find the optimum configuration among four variables pertinent to the ANN which is shown in Table 3.

The parameters include: algorithm of ANN, transfer functions of hidden and output layer and the number of neurons in the hidden layer. It is well known that different algorithms fit different problems. Therefore, choosing an appropriate algorithm is necessary. Details about the training algorithms used in present work are summarized in Table 4. Normally, it is accepted that increasing the number of neurons can enhance the prediction quality of the network. But, this number cannot be increased unlimitedly because one may reach a saturation value, resulting in the over-fitting issues. The best structure was deduced that the optimum configuration has been found out between 1890 numbers of architectures. The training and testing process was repeated hundereds of times in each model to find best weights and biases that cause lowest MAPE and the results of the ANN performance test and were saved in a five dimensional matrix.

TABLE 3. The ANN architecture variables

Number of neurons in hidden layer	**1-30**
Activation function of hidden layer	logsig, tansig, purelin
Activation function of output layer	logsig, tansig, purelin
Training algorithms for back propagation	trainlm, traincgb, trainscg, trainbfg, traingdx, traingda

Then, at the end of run, the resulting matrix was passed through a sort program to find the best architecture with the lowest MAPE. When the program found the optimum architecture in one hidden layer, it was developed for fining of the lowest MAPE in two hidden and three hidden layer with optimum architecture.

3. 2. Results of Modeling and Discussion The results of performed program (Figure 4) show that BFG and LM training algorithm are the best among six algorithms with lowest MAPE. The characteristics of architectures after training by BFG algorithm showed in Figure 5. The MAPEs were scaled with respect to the minimum MAPE found for the optimized architecture and the smaller the radius of the circle showed the less MAPE for that special architecture.

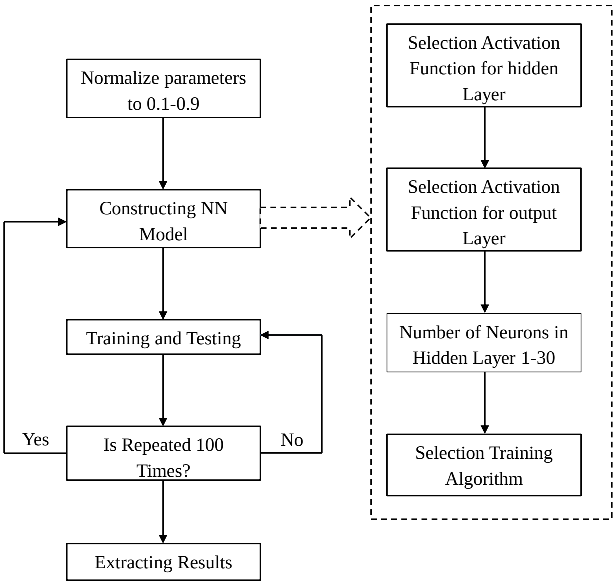

Figure 3. The flowchart of finding suitable the ANN architecture

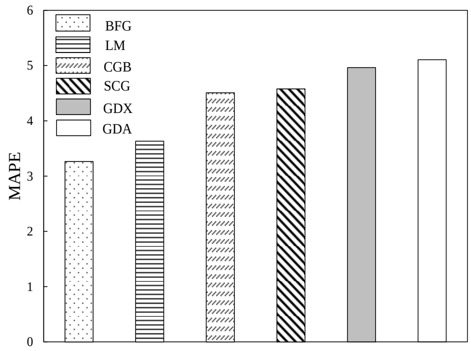

Figure 4. Comparison of (MAPE) for various training algorithms

The final architecture among of structures is 7-[25]-1 with Quasi-Newton method (BFG) algorithm and log-sigmoid transfer function as an activation function for hidden layer and tangent sigmoid for output layer which have 3.26% error.

TABLE 4. The description of the algorithms applied for training of network

Algorithms	Description
LM–Levenberg-Marquardt algorithm	One of the fastest training algorithms for networks of moderate size
CGB–Powell-Beale conjugate gradient algorithm	The converge rate is generally faster
SCG–scaled conjugate gradient algorithm	Combine credible interval method and conjugate gradient algorithm with no line search
BGF–BFGS Quasi-Newton method	Usually converges in fewer iterations but requires to estimate Hessian matric
GDX–adaptive learning rate algorithm	Faster than basic gradient descent algorithm
GDA–adaptive learning rate algorithm	Slower than GDX without momentum

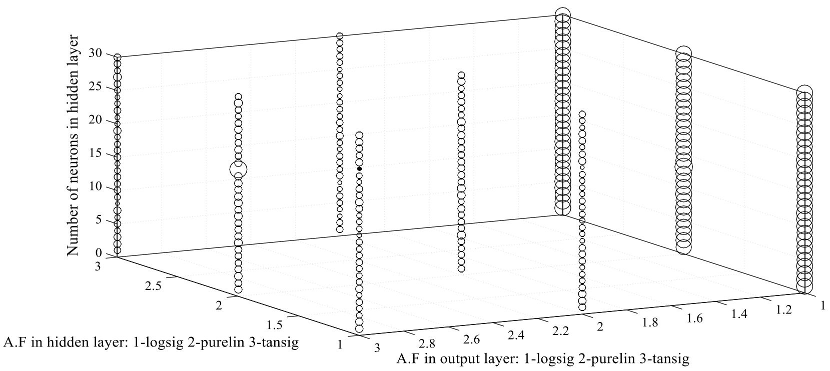

Figure 5. MAPE errors for different architectures using Quasi-Newton method technique for training the networks, the smaller the circles, the better the architecture

The mean absolute percentage error (MAPE), mean square error (MSE), root mean square error (RMSE) and sum of square errors (SSE) of training and testing data sets are shown in Table 5. Based on Figures 6 and 7, the conclusion can be made that the prediction of hardness by neural network is closer to the measured values; the high coefficient of determination values show that the prediction was acceptable. As shown in Figure. 8, by increasing of CNT wt% and milling time, the hardness was increased.

TABLE 5. Actuarial parameters of the ANN model for predicted hardness in different hidden layer

Number of Hidden layer	Data	MAPE	SEE	MSE	RMSE
One	Testing set	3.265	0.00444	0.000247	0.0157
	Training set	4.136	0.00738	0.000305	0.0225

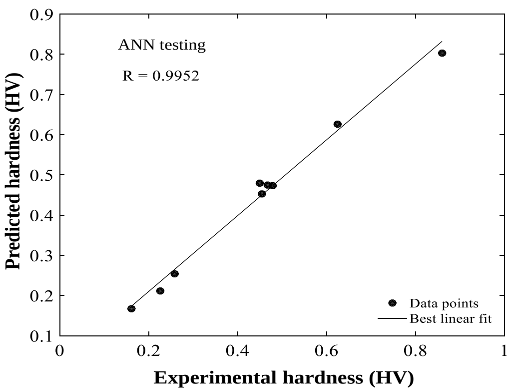

Figure 6(a). Regression analysis of predicted and experimental hardness for testing data

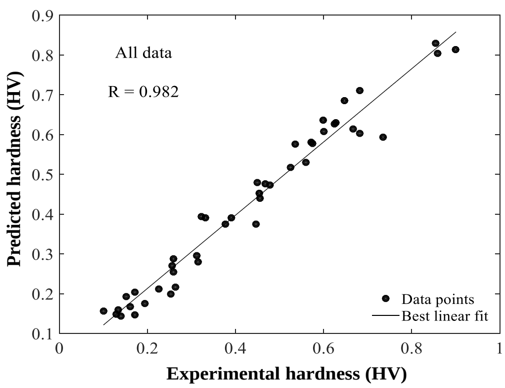

Figure 6 (b). Regression analysis of predicted and experimental hardness for all data

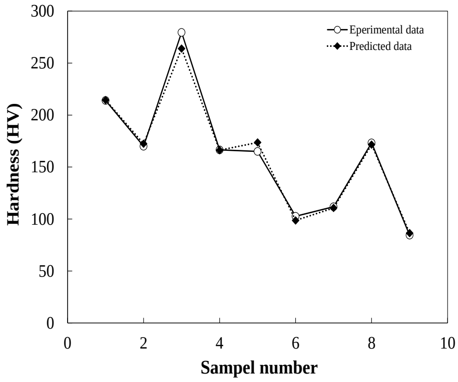

Figure 7. Comparison of experimental hardness with predicted hardness

Moreover, the comparison of Figure 8(a) and 8(b) indicate that the proposed model has relatively good accuracy.

3. 3. Sensitivity Analysis The sensitivity test was conducted to investigate the sensitivity of the model outputs to the input parameters variation. Sensitivity analysis allows an operator to quickly recognize the optimum conditions of input parameters for better selection of appropriate production conditions.

In this analysis, a step-by-step method was carried on the trained ANN by varying each of the input parameters, one at a time, at a constant rate. Various constant rates 5 and 10 were selected in this study. For every input parameter, the percentage was changed in the output as a result of the change in the input parameter. The sensitivity of each input parameter was calculated by the following equation:

$$S_i\left(\%\right) = \frac{1}{N}\sum_{j=1}^{N}\left(\frac{\%change\ in\ output}{\%change\ in\ input}\right)_j \times 100 \qquad (10)$$

where S_i *(%)* is sensitivity level of an input parameter and *N* the number of datasets applied to test the network. Figure 9 indicates the change in hardness with each of the input variables. The results showed that the sintering temperature and amount of MWCNT have the greatest effect, while BPR has comparatively less influence on samples hardness. Also, the sintering temperature shows an adverse effect and the amount of reinforcement has a direct effect on Al2024-CNT nanocomposite hardness. It was realized that by increasing sintering temperature, the tendency of carbon to react with Al matrix and formation of needle shape Al_4C_3 phase was increased and consequently deteriorated the hardness of Al-CNT nanocomposites [8]. In addition, the hardness in Al2024 composite reinforced with CNTs shows a rapid increase with increase of CNT concentration [30].

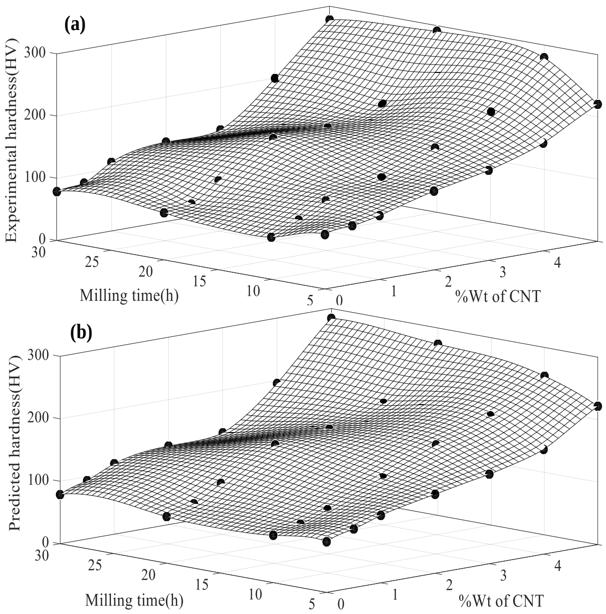

Figure 8. 3D profiles of direct dependence of hardness of Al2024-CNT composite on the amount of CNT and milling time at same parameters (Sintering temperature 550°C, Sintering time 2h, Compact pressure 1500MPa, Vial speed 300rpm and Ball to powder weight ratio:5).

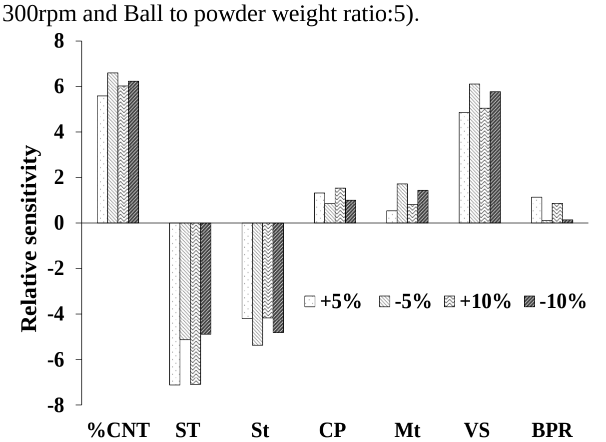

Figure 9. Significance of input parameters on the mechanical properties.

4. CONCLUSION

This work demonstrates the excellent capability of an ANN technique for simulation of mechanical properties of Al2024 reinforced with multiwall carbon nanotubes. In particular, the hardness was predicted by a sufficiently trained neural network based on material compositions and manufacturing parameters as input parameters. The prediction accuracy was satisfactory, but its dependence on the number of training data shows that the accuracy could be further enhanced by extending the experimental database for network training. Furthermore, a well-trained neural network prepares more appropriate data from a relatively limited practical database. This means a considerable saving of cost and time, which could benefit the industry to build more general and specific databases of material properties.

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Mechanical Alloying

چکیده

در این پژوهش از شبکه عصبی مصنوعی به منظور پیش‌بینی میکرو سختی کامپوزیت Al2024 تقویت شده با نانو لوله‌های کربنی چند دیواره ساخته شده به روش آلیاژسازی مکانیکی استفاده شده است. بنابراین، مقدار فاز تقویت کننده، نسبت گلوله به پودر، فشار پرس، زمان آسیاب کاری، دما، زمان تف‌جوشی و سرعت آسیاکاری به عنوان پارامترهای مستقل ورودی و میکروسختی متوسط کامپوزیت به عنوان پارامتر خروجی انتخاب شده‌اند. برای آموزش مدل، از ساختار شبکه عصبی چند لایه پرسپترون و الگوریتم پس‌انتشار خطا استفاده شده است. بعد از امتحان معماری های ANN متفاوت، ساختار مدل بهینه به صورت ۱–۲۵–۷ به دست آمد. نتایج پیش‌بینی شده با نسبت همبستگی بین ۰/ ۹۸۲ و ۰/۹۹۵۲ و ۳/۲۶ درصد خطای میانگین مطلق، سازگاری بسیار خوبی با مقادیر تجربی نشان می‌دهد. علاوه بر این، مدل شبکه عصبی به منظور پیدا کردن اهمیت پارامترهای ورودی موثر بر خواص مکانیکی نمونه‌ها تحت آنالیز حساسیت قرار گرفت.

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