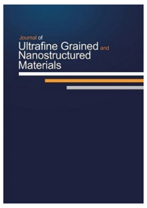


**Journal of Ultrafine Grained and Nanostructured Materials**
https://jufgnsm.ut.ac.ir
Vol. 50, No.1, June 2017, pp. 23-32
Print ISSN: 2423-6845 Online ISSN: 2423-6837
DOI: 10.7508/jufgnsm.2017.01.04

# Hardness Optimization for Al6061-MWCNT Nanocomposite Prepared by Mechanical Alloying Using Artificial Neural Networks and Genetic Algorithm

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*Recieved: 26 October 2016; Accepted: 3 June 2017*

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**ABSTRACT**

Among artificial intelligence approaches, artificial neural networks (ANNs) and genetic algorithm (GA) are widely applied for modification of materials property in engineering science in large scale modeling. In this work artificial neural network (ANN) and genetic algorithm (GA) were applied to find the optimal conditions for achieving the maximum hardness of Al6061 reinforced by multiwall carbon nanotubes (MWCNTs) through modeling of nanocomposite characteristics. After examination the different ANN architectures an optimal structure of the model, i.e. 6-18-1, is obtained with 1.52% mean absolute error and $R^2 = 0.987$. The proposed structure was used as fitting function for genetic algorithm. The results of GA simulation predicted that the combination sintering temperature 346 °C, sintering time 0.33 h, compact pressure 284.82 MPa, milling time 19.66 h and vial speed 310.5 rpm give the optimum hardness, (i.e., 87.5 micro Vickers) in the composite with 0.53 wt% CNT. Also, sensitivity analysis shows that the sintering time, milling time, compact pressure, vial speed and amount of MWCNT are the significant parameter and sintering time is the most important parameter. Comparison of the predicted values with the experimental data revealed that the GA–ANN model is a powerful method to find the optimal conditions for preparing of Al6061-MWCNT.

***Keywords:*** *Carbon nanotubes; Metal–matrix composites; Genetic algorithm; Artificial neural network.*

*How to cite this article:*
*Mahdavi Jafari M, Soroushian S, Khayati GR. Hardness Optimization for Al6061-MWCNT Nanocomposite Prepared by Mechanical Alloying Using Artificial Neural Networks and Genetic Algorithm. J Ultrafine Grained Nanostruct Mater, 2017; 50(1):23-32.*
*DOI: 10.7508/jufgnsm.2017.01.04*



## 1. Introduction

Since the original work of Iijima in 1991 [1], carbon nanotubes (CNTs) have been recognized to possess outstanding attributes [2], in particular in the area of nanotechnology. One of the most important usages of CNTs is in the production process of composites, where CNTs are applied as new reinforcement and binders to enhance the mechanical, electrical and thermal properties [3–5]. CNTs have high potential usage due to their very large aspect ratio (1000–10,000) [6], low density, high rigidity (Young's modulus of the order of 1TPa) [7–8] and high tensile strength (up to 60 GPa) [9]. In addition, the thermal conductivity of multiwalled carbon nanotubes (MWCNTs) was assigned to be >3000 W/mK [10], making them suitable selection in preparing composites with improved properties. However, most researches are carried out on CNTs/polymer composites [11–13] which indicate a tremendous strengthening effect for the composites. Therefore, CNTs–metal matrix composites are also expected to notice the role of structural materials.

In the field of metal-matrix composites, Al composites have been paid so much attention due to their wide usage in industries because of their light weight, high strength as well as good corrosion resistance. However, no important breakthrough has yet been made on CNTs-reinforced Al matrix composites. Especially the obstacles associated with the interfacial bonding between CNTs and Al matrix and lack of suitable synthesis method to gain a homogenous dispersion of CNTs and Al matrix. This is mostly because of the strong van der Waal's force of attraction between them leading to agglomeration rather than dispersion. Therefore, the development of bulk fabrication procedure for Al–CNTs composite was started on the basis of a mechanical milling procedure [14, 15] to find a uniform distribution of CNTs in Al matrix. Mechanical milling is a solid-state high-energy ball milling method where particles are repeatedly fractured and welded [16] and has been applied to disperse uniformly a variety of reinforcement materials within Al matrix [17]. Few other processes that have been applied are roll-bonding followed by annealing [18], plasma spray forming [19], liquid infiltration [20] and high pressure torsion [21]. To the best of our knowledge, the powder metallurgy was an appropriate method for producing MWCNTs reinforced Al-matrix composites [22–24]. This procedure mostly consists of mechanical milling of MWCNTs with Al powder either in dry or wet situations followed by compaction and sintering.

An engineering technique to optimize the process factors is based on the utilization of artificial neural network and genetic algorithm. Artificial neural network is a powerful non-linear strategy for simulation of complicated materials behavior [25]. This strategy can learn and predict the experiential knowledge with setting the weight and bias in neuron but cannot determine the optimum condition and might be hampered in the local minimum. Genetic algorithm (GA) is a population-based evolutionary search and optimization process, which needs the definition of a selection, a crossover and a mutation of genetic information, to evolve into the next generations with potentially solutions of a particular problem. The present study was carried out using combined GA-ANN due to their flexibility over the general regression processes to determine a suitable process conditions for Al6061-MWCNT nanocomposite. To confirm the predictions of GA, the Al6061-MWCNT samples were made as presented by GA condition.

## 2. Artificial Neural Network Modeling

Among artificial intelligence approaches, artificial neural networks (ANNs) are widely employed and are some of the powerful method for problems in many spheres [26-27]. ANNs are consist of numerous of interconnected nonlinear memory less processing elements called neurons. The neurons of each layer are linked to that of the next layer through associated weights. The network applies the information of these weights to solve the problems. A connected neuron formula is presented as (eq. 1):

$$x = \sum_{i=1}^{p} w_i x + b \qquad \text{(eq. 1)}$$

Where $b$ shows the bias of neurons, $p$ presents the number of elements and $w_i$ is the weight of the input vector *xi*. Each neuron receives the sum of the weight inputs with bias and employs the activation function to confirm its output signal, as presented in (eq. 2):

$$f(x) = f\left(\sum_{i=1}^{p} w_i x + b\right) \qquad \text{(eq. 2)}$$

Where the transfer function (f) of the neuron shows the hyperbolic tangent sigmoid (tansig) activation function (Fig.1), which in the present study is given as (eq. 3):

$$f(x) = \frac{exp(x) - exp(-x)}{exp(x) + exp(-x)} \qquad \text{(eq. 3)}$$

Between neural network techniques, feed-forward back-propagation (BP) neural network is

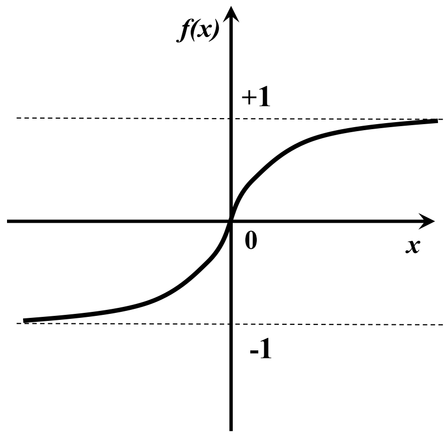

Fig. 1- Shape of hyperbolic tangent sigmoid (tansig) function.

extensively applied to presenting effective solutions in the engineering applications especially in material science [28-30]. BP learning is based on the difference between the output value determined by the model and the desired value to improve the interconnection values, which include the weights and the biases of the processing neurons. A BP network includes one input, one or two hidden, and one output layers.

Based on the investigation by Hornick, Stinchcombe, and White [31-33], one to two hidden layers could show appropriate training results. The typical feed-forward $ANN_S$ are presented in Fig. 2. Before applying a feed-forward BP network, the architecture of the network has to be set because it affects the performance of the network, significantly. Five factors, including the number of hidden layer and neurons, the learning method, and activation function for hidden layer and output layer are the characteristics of an ANN structure. Usually, the determination strategy of these network factors is trial and error. To determine the best architectures of feed-forward back propagation ANN a program was developed to train and evaluate the various architectures with a various number of neurons in one hidden layer (1 up to 30) while, other parameter is fixed. In this paper used Levernberg-Marquardt algorithm (LM) as training strategy while hyperbolic tangent sigmoid (tansig) as activation function in the hidden layer and output layer. Fig. 3 shows the program flowchart. Developing a BP network model involves applying a large number of training sets and training cycles to adjust the weight and the bias of each neuron.

The hardness of Al6061-MWCNT nanocomposite that prepared by mechanical alloying and sintering is a function of average diameter of CNT, average length of CNT, average metal particle size, amount of reinforcement compaction pressure, milling time, sintering temperature, sintering time, vial speed. These features were chosen as input variables in ANN model while the hardness of nanocomposite was the output parameter. In order to ANN modeling, a database containing 46 various independent hardness experiments of Al6061-CNT nanocomposites collected from different works [34-37], where 37 and 9 group of data randomly selected for train and validate, respectively. Table 1 displays the statistical information of the developed database. In this paper, the minimal mean-absolute-percentage-error (MAPE) of the training and testing sets has been anticipated. MAPE is determined as the average absolute error between the predicted outputs of the established network and the target outputs (given as (eq. 4)):

$$MAPE = \frac{1}{L}\left[\sum_{i=1}^{L} \frac{|T_i - P_i|}{T_i}\right] \times 100 \qquad \text{(eq. 4)}$$

Where $L$ displays the number of samples, $T_i$ is the actual output value of sample $i$, and $P_i$ is the predicted output value of sample $i$. Usually, the smaller the MAPE, the more acceptable the

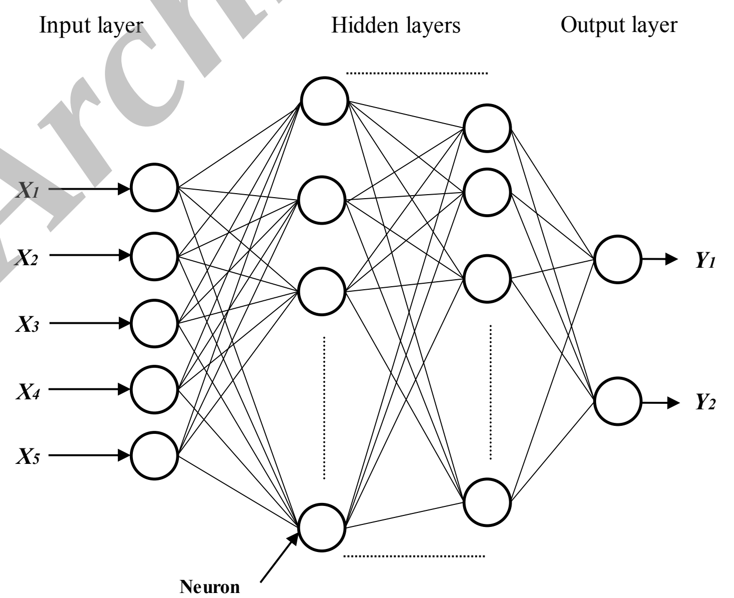


Fig. 2- Typical feed-forward neural networks.

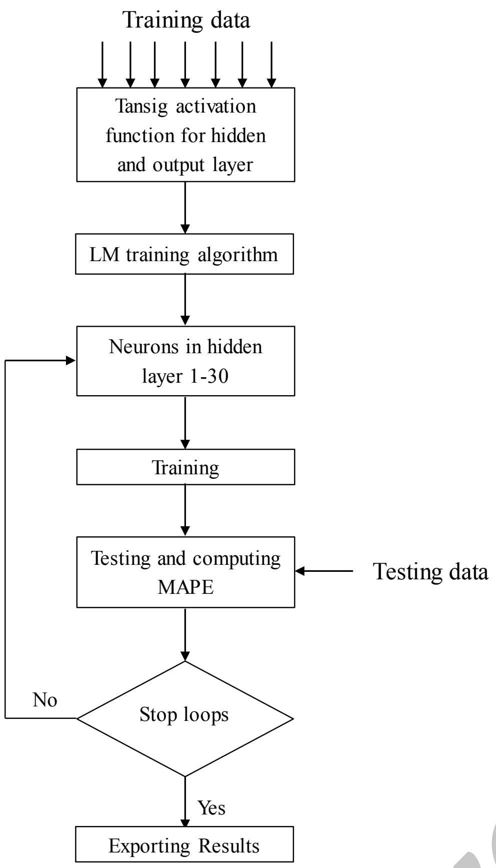


Fig. 3- The flowchart of finding suitable the ANN architecture.

constructed network is. After repeated training, the relationship between the inputs and the predicted outputs might be determined to meet the actual outputs via the functional model of the neural network.

### 3. Genetic Algorithm (GA)

GA is the search strategy based on the mechanics of natural selection and natural genetics to discover the best solution for specific environment or problem conditions [38]. GA starts with generating random initial population consisted of potential solution points (or individuals). The value set for each individual from the evaluation procedure with objective function is named the fitness. The decision is made whether the individual is good or bad for the particular problem, based on the magnitude of fitness value. Once fitness value is tested and assigned to each individual, then the initial population meets the first genetic operator, selection procedure.

The purpose of this step is to give more chances of survival for the strong individuals and to die off the weakest ones according to their fitness values. Next, crossover operator is done on selected individuals to generate the new individuals by combination of the existing ones [39]. Crossover performs reproduction and allows two individuals to exchange portions of their structures based on a particular probability. Which chromosomes to cross and where to cut them is performed statistically based on a particular probability. This results in the creation of a pair of new chromosomes that contain features of their parents [40, 41]. This process can be compared to the natural evolution procedure generating new children from the parents. Finally, the mutation operator follows the crossover procedure. Mutation operators for the real-valued representation have been proposed by Michalewicz [42]. The major role of mutation procedure is to present the diversity in the population. Without

Table 1- The statistical information of the developed datasets

| Parameters | Maximum | Minimum | Average | Standard deviation |
|---|---|---|---|---|
| **Input variable** | | | | |
| Amount of reinforcement (wt. %) | 2 | 0 | 0.84 | 0.68 |
| Sintering temperature (°C) | 640 | 30 | 472.93 | 176.36 |
| Sintering time (h) | 2 | 0.33 | 1.09 | 0.8 |
| Compact pressure (MPa) | 500 | 35 | 240.76 | 229.95 |
| Milling time (h) | 30 | 0.5 | 13.84 | 14.33 |
| Vial speed (rpm) | 1200 | 200 | 473.91 | 413.03 |
| **Output variable** | | | | |
| Hardness (HV) | 87.5 | 48.2 | 62.63 | 8.34 |

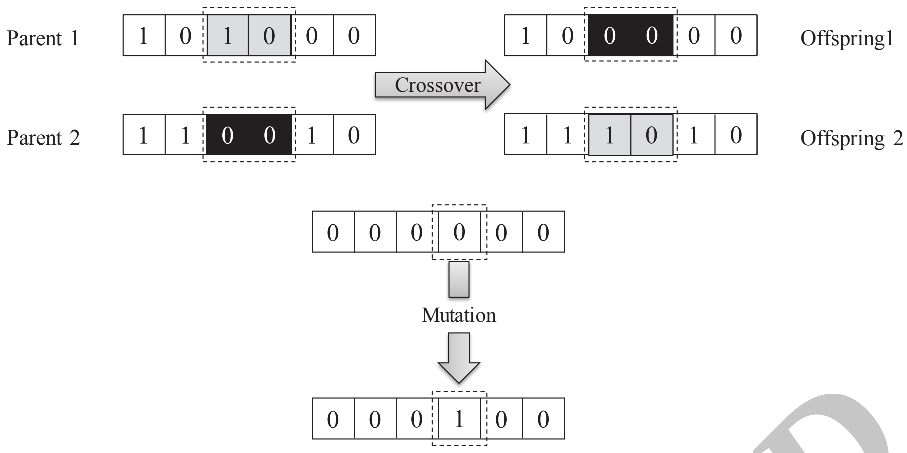


Fig. 4- Illustration of the GA operations.

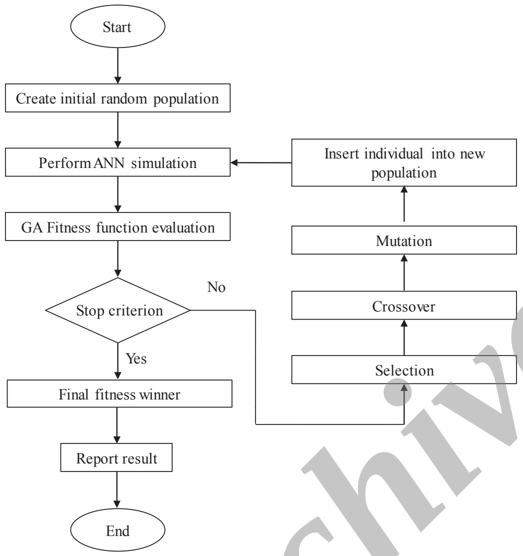


Fig. 5- Optimization process based on ANN and GA.

the mutation, it is hard to obtain the solution point that is located far from the current direction of search. It insures that the probability of obtaining any point in the search space never go to zero [43]. This operator also prevents the premature convergence of GA to one of the local optimal solutions. Once all three main operators are done on the initial population, the new population is developed. This new population is genetically superior to the previous one and has better chance to survive for the given problem features. Then this entire procedure is repeated until the satisfaction is obtained or it reaches the maximum number of generations which is pre-set by users. Fig. 4 presents the genetic algorithm operator procedure in simplicity.

## 4. The Combined GA–ANN Model

The following stage involves the development of the GA population of the input parameters for utilization in the probabilistic based optimum search. This is followed by the prediction the system outputs using an ANN model of the system [44, 45]. For mechanical features of Al6061-MWCNT nanocomposite in this investigation, the fitness function commonly addresses higher hardness in ANN model. Once the outputs are determined through the ANN computation, the relevant outputs are exerted to the fitness function routine to set the latest values and compared. While, the fitness requirements are being adjusted from time to time, a new generation of the population will be generated and gone through the same evaluation procedures. This procedure continues until the maximum number of generation has been obtained. The final population of the generation is defined the "winner" and rewarded the conclusive generation of final fitness. Fig. 5 introduces a summary outline of the optimization plan. GA and ANN methods were implemented in MATLAB software (version 2014b).

## 5. Results And Discussion

The ANN modeling program results show that the best ANN structure has 18 neurons in hidden layer with 1.52% error among 30 structures, as shown in Fig. 6. The predicted values, deviation and % error for the hardness is presented in Tables 2 and 3 and a comparative plot of real and predicted values for training and testing is presented in Fig. 7. The close linear trend between the ANN predicted and experimentally observed values for the output parameters indicate the adjacency of the model

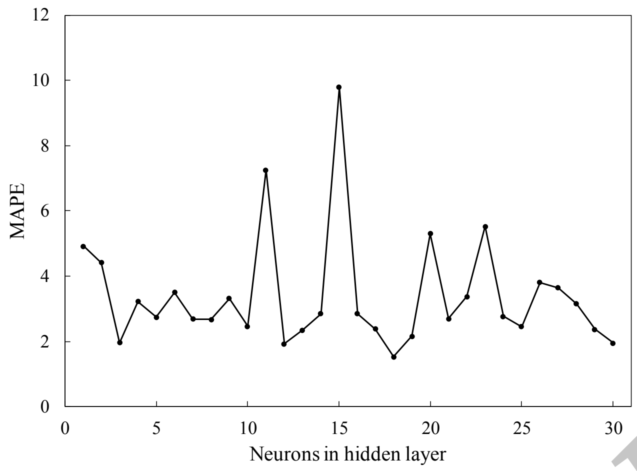


Fig. 6- Amount of error for different ANN structure.

Table 2- Experimental data and predicted output from the ANN network for training set

| | Amount of MWNCT (wt. %) | Sintering temperature (°C) | Sintering time (h) | Compact pressure (MPa) | Milling time (h) | Vial speed (rpm) | Hardness (HV) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | Measured | Predicted | Error |
| 1 | 0 | 30 | 2 | 500 | 30 | 280 | 52 | 52.01 | -0.01 |
| 2 | 1 | 640 | 0.5 | 50 | 3 | 1200 | 76.5 | 78.02 | -1.52 |
| 3 | 0 | 525 | 2 | 500 | 30 | 280 | 55 | 55.01 | -0.01 |
| 4 | 1 | 640 | 0.5 | 50 | 1 | 1200 | 60.4 | 56.78 | 3.61 |
| 5 | 0.5 | 30 | 2 | 500 | 30 | 280 | 53 | 52.59 | 0.4 |
| 6 | 0.5 | 400 | 0.33 | 35 | 1 | 200 | 59.1 | 59.18 | -0.08 |
| 7 | 1.5 | 30 | 2 | 500 | 30 | 280 | 60 | 60.86 | -0.86 |
| 8 | 0 | 640 | 0.5 | 50 | 3 | 1200 | 62 | 61.66 | 0.33 |
| 9 | 1 | 450 | 2 | 500 | 30 | 280 | 59 | 58.89 | 0.1 |
| 10 | 1.5 | 450 | 2 | 500 | 30 | 280 | 62 | 61.97 | 0.02 |
| 11 | 2 | 450 | 2 | 500 | 30 | 280 | 66 | 65.42 | 0.57 |
| 12 | 1 | 640 | 0.5 | 50 | 2 | 1200 | 71.1 | 68.51 | 2.58 |
| 13 | 1 | 525 | 2 | 500 | 30 | 280 | 61 | 61.02 | -0.02 |
| 14 | 1.5 | 525 | 2 | 500 | 30 | 280 | 66 | 66.03 | -0.03 |
| 15 | 0.5 | 500 | 0.33 | 35 | 1 | 200 | 65.7 | 65.55 | 0.14 |
| 16 | 0.5 | 600 | 2 | 500 | 30 | 280 | 58 | 56.89 | 1.1 |
| 17 | 1 | 600 | 2 | 500 | 30 | 280 | 62 | 62.01 | -0.01 |
| 18 | 0 | 640 | 0.5 | 50 | 3 | 1200 | 61.5 | 61.66 | -0.16 |
| 19 | 2 | 600 | 2 | 500 | 30 | 280 | 76 | 75.98 | 0.01 |
| 20 | 2 | 500 | 0.33 | 35 | 1 | 200 | 68 | 67.86 | 0.13 |
| 21 | 1 | 640 | 0.5 | 50 | 0.5 | 1200 | 49.3 | 52.98 | -3.68 |
| 22 | 0.75 | 450 | 0.33 | 35 | 1 | 200 | 67.6 | 67.6 | 0 |
| 23 | 0 | 400 | 0.33 | 35 | 1 | 200 | 56.8 | 60.73 | -3.93 |
| 24 | 0 | 600 | 2 | 500 | 30 | 280 | 57 | 57.17 | -0.17 |
| 25 | 1 | 500 | 0.33 | 35 | 1 | 200 | 69.3 | 69.29 | 0 |
| 26 | 1 | 400 | 0.33 | 35 | 1 | 200 | 63.3 | 63.52 | -0.22 |
| 27 | 2 | 400 | 0.33 | 35 | 1 | 200 | 53 | 52.8 | 0.19 |
| 28 | 0 | 450 | 0.33 | 35 | 1 | 200 | 66.3 | 67.16 | -0.86 |
| 29 | 0.75 | 400 | 0.33 | 35 | 1 | 200 | 60 | 59.8 | 0.19 |
| 30 | 0 | 640 | 0.5 | 50 | 1 | 1200 | 53.2 | 49.83 | 3.36 |
| 31 | 1 | 450 | 0.33 | 35 | 1 | 200 | 71.3 | 70.75 | 0.54 |
| 32 | 2 | 450 | 0.33 | 35 | 1 | 200 | 59 | 59.21 | -0.21 |
| 33 | 0 | 500 | 0.33 | 35 | 1 | 200 | 70 | 69.88 | 0.11 |
| 34 | 1 | 30 | 2 | 500 | 30 | 280 | 57 | 57.05 | -0.05 |
| 35 | 0.75 | 500 | 0.33 | 35 | 1 | 200 | 66.1 | 66.31 | -0.21 |
| 36 | 1 | 620 | 0.5 | 50 | 3 | 1200 | 87.5 | 80.63 | 6.86 |
| 37 | 2 | 30 | 2 | 500 | 30 | 280 | 62 | 63.4 | -1.4 |
| | **MAPE** | | | | | | **1.44** | | |

Table 3- Experiment data and predicted output from the ANN network for testing set.

| | Amount of MWNCT (wt. %) | Sintering temperature (°C) | Sintering time (h) | Compact pressure (MPa) | Milling time (h) | Vial speed (rpm) | Hardness (HV) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | Measured | Predicted | Error |
| 1 | 0 | 640 | 0.5 | 50 | 0.5 | 1200 | 48.2 | 49.49 | -1.29 |
| 2 | 1.5 | 600 | 2 | 500 | 30 | 280 | 68 | 68.78 | -0.78 |
| 3 | 0 | 640 | 0.5 | 50 | 2 | 1200 | 55.5 | 52.61 | 2.88 |
| 4 | 0.5 | 525 | 2 | 500 | 30 | 280 | 56 | 56.28 | -0.28 |
| 5 | 0 | 450 | 2 | 500 | 30 | 280 | 54 | 53.26 | 0.73 |
| 6 | 0.5 | 450 | 2 | 500 | 30 | 280 | 55 | 55.02 | -0.02 |
| 7 | 2 | 525 | 2 | 500 | 30 | 280 | 71 | 71.66 | -0.66 |
| 8 | 0.5 | 450 | 0.33 | 35 | 1 | 200 | 67 | 66.55 | 0.44 |
| 9 | 1 | 600 | 0.5 | 50 | 3 | 1200 | 83.3 | 82.29 | 1 |
| | **MAPE** | | | | | | 1.**52** | | |

with the experimental dataset.

The sensitivity analysis was carried out to set the relative significance of each of the input parameters. The aim of the analysis was to decrease the number of input parameters should they prove to be insignificant in model performance. The reduction of input parameters would result in a decrease in unnecessary data collection, which leads to cost reduction. A step-by-step method was executed on the trained ANN by changing each of the input parameter, one at a time, at a constant rate. Different constant rates (5, 10) were chosen in this paper. For every input parameter, the percentage was modified in the output as a result of the change in the input parameter. The sensitivity of each input parameters was computed by the following equation [46]:

$$S_i(\%) = \frac{1}{N}\sum_{j=1}^{N}\left(\frac{\%change\ in\ output}{\%change\ in\ input}\right)_j \times 100 \qquad \text{(eq. 5)}$$

Where $S_i$ *(%)* shows the sensitivity level of an input parameter and N (= 9) is the number of datasets used for sensitivity test. Fig. 8 presents the sensitivity of variations for mechanical properties at each of the input variables. It can be seen that the sintering time and milling time are the two most important factors. This analysis showed that sintering temperature and sintering time has a reverse effect on the hardness of Al6061-CNT nanocomposite. The former researches showed that the tendency of the reaction of carbon nanotubes with Al6061 and formation of $Al_4C_3$ is ascending by increasing the time and temperature of sintering. The presence of small amount of carbide at the interface of the CNT and matrix can improve the interfacial bonding but excessive carbide formation can result in overall degradation of the composite strength since the carbides have inferior properties compared with the CNTs. Furthermore, this could excessive when milling time is high [47, 48]. Milling time, vial speed, compact pressure and amount of MWCNT have positive effect on hardness. Increasing in milling time and vial speed makes MWCNTs uniformly and completely embedded in

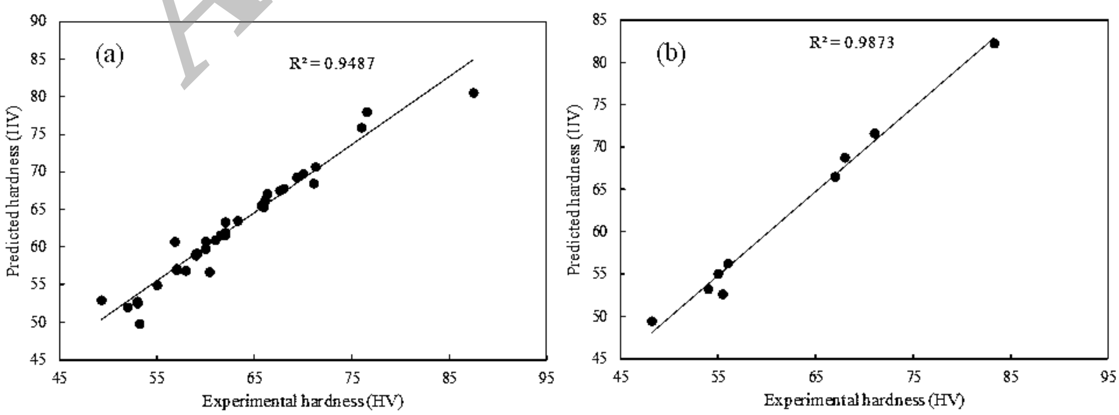


Fig. 7- Regression analysis of predicted and experimental hardness for best structure: (a) Training data; (b) Testing data.

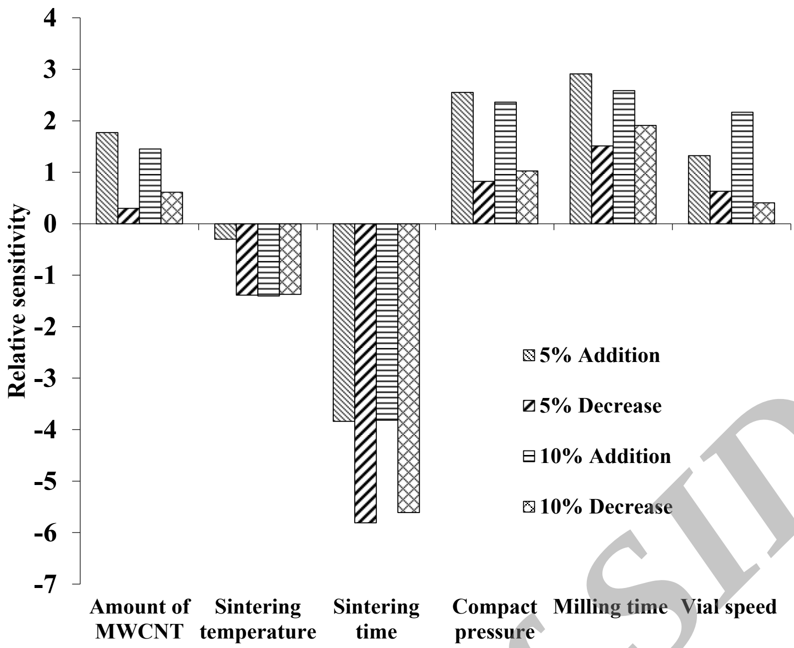


Fig. 8- Significance of input variables in mechanical properties.

the Al 6061 matrix and tighter bonding between the CNTs and Al 6061 which enhances the mechanical properties of the matrix [49]. Also, compact pressure influences green density of the samples which can lead to increase in sintering degree [34].

In this study, genetic algorithms with a single point crossover and roulette wheel selection have been applied. Each individual was produced with a fitness function, which was determined from ANN model. The initial population was selected to be 30, generation size 100 and the probability of crossover and probability of mutation were selected to be 0.8 and 0.2, respectively. GA simulation predicted the combination sintering temperature 346 C, sintering time 0.33 h, compact pressure 284.82, milling time 19.66 and vial speed 310.5 to give optimum hardness of 87.5 micro Vickers in the composite with 0.53 wt% CNT. For evaluating the results, experiments were carried out at different configurations, results of which are summarized in Table 4. The optimum fitness function obtained experimentally was at condition of number 2 which was close to the conditions predicted by GA. This conclusively proves the validity of the simulated results.

## 6. Conclusion

The following conclusions are drawn from this work. ANN model with 18 neurons in hidden layer is a useful method for the prediction of hardness of Al6061 reinforced by multiwall carbon nanotubes where fabricated by mechanical alloying. The combined GA–ANN algorithm is an effective model for optimizing mechanical alloying parameters leading to maximum hardness in Al6061-MWCNT nanocomposite. Sensitivity analysis shows that the sintering time and milling time are most significant parameter and sintering time is the most important parameter among the experimental parameters used in this work.

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TABLE 4. Results of ANN-GA program and experimental validation of optimized value

| | Amount of MWCNT (wt %) | Sintering temperature (°C) | Sintering time (h) | Compact pressure (MPa) | Milling time (h) | Vial speed (rpm) | Hardness (HV) | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | Measured | Predicted |
| 1 | 0.65 | 414.43 | 0.35 | 57.76 | 23.88 | 446.39 | 78.3 | 87.5 |
| 2 | 0.53 | 346.55 | 0.33 | 284.82 | 19.66 | 310.49 | 86.55 | 87.5 |
| 3 | 0.25 | 399.56 | 0.53 | 35.53 | 23.82 | 274.44 | 62 | 87.5 |

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