Prediction of wear properties of graphene-Si$_3$N$_4$ reinforced titanium hybrid composites by artificial neural network

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Abstract

In this study, we have employed artificial neural network (ANN) method to predict wear properties of titanium hybrid composites produced by powder metallurgy (PM) method. Titanium (Ti) was used as a matrix materials and graphene nano-platelets (GNPs)-Si$_3$N$_4$ were used as reinforcement materials in hybrid composites. A back-propagation neural network with 3–6–1 architecture was developed to predict wear rates by considering weight fraction reinforcements, load and density as model variables. The well trained ANN system predicted the experimental results in a good agreement with the experimental data. This refers that ANN can be used to evaluate wear rate of samples in a cost effective way.

1. Introduction

Two dimensional compounds were hypothetical objects until 2004 when graphene was isolated [1]. One of the important reason for nonexistence of two dimensional compounds was thermal instability when they were seperated. Graphene is a crystal that has a two-dimensional structure made of carbon atoms. It is the essential structural element for other allotropes, such as carbon nanotubes and fullerenes. Therefore graphene plays an important role in understanding the electronic properties of other allotropes [2].

Carbon atoms have four electrons on valence shell and these electrons are responsible for chemical bonding. In graphene, being a two dimensional structure, each carbon atom is bonded to the three carbon atoms. As a result of this connection, an electron is ‘liberated’ for electronic conduction. In this manner, graphene is an important playground since it is the basis for the understanding of the electronic properties of materials. For example, for an ordinary particle in classical and non-relativistic quantum mechanics, energy of the any particle $E$ is proportional to the square of the momentum, $p^2$, i.e. $E \sim p^2$. This means that Schrödinger equation can be used for these systems. On the surface of graphene, the energy of the electron is linear in momentum, $E \sim p$, where Dirac equation can be used. For the time being, graphene is the only material on which Dirac equation can be experimentally studied. Besides that electron flow resembles the motion of the relativistic Dirac particles [2].

Nowadays, graphene has became a hot topic in physics and engineering studies due to its extraordinary properties such as optical [3–5], strength [6–9], electricity [10–12], and heat conduction [13–16].

Due to their main properties like high strength, low density and higher corrosion resistance, titanium (Ti) became one of the most important engineering materials. Based on these properties, pure Ti is being used as a matrix material in the composites [17–20]. In recent years carbon based materials, especially graphene nanoplates (GNPs) are the most preferred materials due to the its remarkable properties. GNPs can be used as a reinforcement material in Ti matrix composites. Moreover, there are many studies about this topic in the literature, for example [21–25]. This kind of composites have many application areas such as biomaterials, aerospace and automotive industries.
One of the most interesting subjects of recent years for new materials is hybrid composites. They are composites which have a combination of two or more reinforcement materials. The usage of composite materials for engineering applications has been impeded by the significant expense of the producing component [26]. Simulation of material properties can be helpful in the optimization. The absence of useful methods to predict material properties for understanding basis of particulate reinforced composites is a challenging task. Furthermore nonlinear behaviour, like in wear process, of the problem makes this task more untouchable. Therefore artificial neural networks (ANNs) has been used in material science for modeling physical and mechanical properties of engineering materials [27–35].

ANNs are information processing systems or computational models based on biological nervous system. This approach stems from the problem solving process of human brain. It is a mathematical tool that mimickes human brain functions [36–39]. ANN methods have been used as powerful techniques to solve a diverse of real-world problems since they have excellent learning capacity. This method can be very helpful with legitimate care and adequate data for simulations of any correlation.

In the present study, we studied wear behaviour of GNPs and Si3N4 reinforced Ti-matrix hybrid composite which was produced in [40] by Artificial Neural Network (ANN) method. These reinforcements materials (GNPs and Si3N4) are used in Ti-matrix for producing hybrid composites by powder metallurgy (PM) method which is a new study for literature.

The paper organized as follows: in section 2, ANN framework is presented. In section 3 the process of composite production and in section 4 neural network setup are given. In section 5, both experimental and ANN results are presented. In section 6, the conclusion of this work is given.

2. Artificial neural network framework

Artificial neural networks are considered to be a model of human brain. The structure of networks consists of highly interconnected processing units which are called neurons. They are arranged in different layers in the neural network and connected each other by weighted links (adaptive synaptic weights) over which signals can pass.

There are three layers in the neural network structure: input layer, hidden layer and output layer. Input layer provide information from the outside world to the network. They receive data from outside. The formal job is done in input layer is to transfer the data to the other layers. There is no computation in this layer. In the hidden layer, information is transferred from the input layer to the output layer. At the same time computations are made. In the output layer, the result of the computational process are displayed to the outside world. A schematic diagram of an ANN is showed in figure 1.

Figure 1 is an example of feed forward neural network in which information moves in only one direction, forward from the input layer to the output layer.

ANNs consist of several neurons and they are the fundamental processing units in a network. They are connected each other over adaptive synaptic weights. Each neuron in the different layers receives one or more input over these connections and produces only one output. This output can be spread to the other neurons in the network.

The mathematical architecture of an ANN can be seen in figure 2.

In a single artificial neuron, the main components are synaptic weights, threshold (addition) function, activation function and outputs. Inputs $x_i$ are obtained from outside the neuron by experimental data. They can
be any data related to the problem. Synaptic weight \( w_{ij} \) refers to the strength of a connection between two neurons in different layers. In general, these weights are taken as random numbers. A function \( f(s) \) acts on the produced weighted signal. This function is called activation function.

The output of the \( i \)th neuron \( N_i \) is
\[
O_i = f \left( w_0 + \sum_{j=1}^{n} w_{ij} x_j \right). \tag{2.1}
\]

The neuron’s work condition can be defined as
\[
w_0 + \sum_{j=1}^{n} w_{ij} x_j \geq \Theta, \tag{2.2}
\]
and the input of the \( i \)th neuron \( N_i \) is
\[
s_i = w_0 + \sum_{j=1}^{n} w_{ij} x_j. \tag{2.3}
\]

The output signal obtained by activation function is
\[
O_i = f \left( s_i - \Theta_i \right), \tag{2.4}
\]
where \( \Theta_i \) is a threshold value which has to be reached or exceeded for the neuron to produce output signal. All the inputs are multiplied by their synaptic weights and added together to form the net input to the neuron. This is called net and written as
\[
net = \sum_{j=1}^{n} w_{ij} x_j + \Theta \tag{2.5}
\]
where \( \Theta \) is a threshold value which is added to the neurons. The neuron takes these inputs and produce an output \( y \) by mapping function \( f(\text{net}) \)
\[
y = f(\text{net}) = f \left( \sum_{j=1}^{n} w_{ij} x_j + \Theta \right) \tag{2.6}
\]
where \( f \) is the neuron activation function. A sigmoid function of the form
\[
y = f(\text{net}) = \frac{1}{1 - e^{-\text{net}}} \tag{2.7}
\]
is the most common activation function since it is useful in linear and nonlinear problems.

The solution of an engineering problem or any other computation like image processing in ANN is based on learning through examples. ANN learns by examples and acquire knowledge about the problem or system. Learning is done by training the network with adequate data set. The important point in this mechanism is that neural network can learn by examples without having known any formulae about the problem or system. By
Table 1. Composite designation.

| Hybrid Composite Sample | GNPs reinforcement | Si₃N₄ reinforcement |
|-------------------------|-------------------|-------------------|
| Pure Ti                 | —                 | —                 |
| TiSG15 0.15 wt% 3 wt%   |                   |                   |
| TiSG30 0.30 wt% 3 wt%   |                   |                   |
| TiSG45 0.45 wt% 3 wt%   |                   |                   |
| TiSG60 0.60 wt% 3 wt%   |                   |                   |

doing this, like in human brain, it can generalize some knowledge which could be used for in the solution process. If the training process is done appropriately, the neural network can gain ability to solve unknown or unfamiliar instances of the problem or system. It should be also noted that the learning mechanism from small experimental data makes ANNs important for manufacturing issues.

3. Materials details and wear test

One of us (T Mutuk) [40] have studied about hybrid composites which were produced with powder metallurgy (PM) method. Titanium (Ti) was used as a matrix materials and GNP-Si₃N₄ were used as a reinforcement materials in hybrid composites. The matrix material was chosen as pure Ti powder (Alfa Aesar, −325 mesh) and also reinforcement materials were chosen graphene nano platelets (GNPs) (Grafen Chemical Industries Co.) and Si₃N₄ (Ube Ind., <1 μm). Different percentages of GNP and Si₃N₄ added in the composite by weight of titanium. GNP reinforcements of 0.15 wt%, 0.30 wt%, 0.45 wt% and 0.6 wt% and other reinforcement material Si₃N₄ of 3 wt% were mixed with pure Ti powder. These properties can be seen in table 1. The synergic effect of GNP-Si₃N₄ particles on density, wear rate and microstructure of hybrid composites were studied [40].

Graphene has major properties on mechanical and microstructure in the composite. One of these is the solid lubricant properties of graphene. This feature has an effect on wear properties on composite. When the graphene in the composite touches with the abrasive counter part during wear test, it prevents the delamination of composite because of solid lubricant properties [41–43]. Besides, Si₃N₄ has mechanical properties, corrosion resistance and abrasion resistance are better than many high strength ceramic materials at high temperatures. Therefore, these kind of materials were selected for producing hybrid composite in this study.

In this study, we have employed artificial neural network (ANN) method to predict wear properties of titanium hybrid composites. Titanium (Ti) was used as a matrix materials and Graphene nano-platelets (GNPs)-Si₃N₄ were used as a reinforcement materials in hybrid composites. Wear tests conditions in this study were performed using a pin-on-disc wear test unit at ambient temperature under dry conditions. The material of the counterpart disc consists of stainless steel with a radius of 20 mm, and a hardness of 65 HRC. Moreover, hybrid composite samples were produced 10 mm radius and 3 mm thickness for wear tests [40, 44].

During the wear test different loads (10 N, 20 N, 30 N) were carried out on the composite. The sliding distance (L) was calculated according to equation (2.8)

\[
L = \frac{2\pi nt}{V m} \tag{2.8}
\]

\[
\Delta V = \frac{\Delta m}{\rho} \tag{2.9}
\]

\[
W = \frac{\Delta V}{PL} \tag{2.10}
\]

where L is the sliding distance (500 m), R is the radius of counterpart disc (20 mm), n is the number of revolutions (200 rpm) and t is the testing time (20 min). The volume change of worn samples (\(\Delta V\), equation (2.9)) were measured using by mass loss (\(\Delta m\)) and density of composite (\(\rho\)). The wear rates (W) of composites were calculated by equation (2.10), where W, P are the wear rate (mm³/(N·m)) and applied load (N), respectively [44].

Figure 3 shows the SEM micrographs of hybrid composites after wear testing at a load of 30 N. At this wear testing conditions, a minimum wear rate of TiSG15 was observed. These images give the highest damage, deepest wear groove and a lot of deep pits for pure Ti. Less damage and groves are observed in the surface of the TiSG15 hybrid composite (figure 3(a)). As expected, the depth of grooves and wear rate increased with increasing load. GNP and Si₃N₄ have uniform distributions in the Ti matrix without agglomeration up to 0.15 wt% GNP content. Moreover, the agglomeration of GNP occurs using a large amount of GNPs. As seen in (figure 3(c)) agglomeration and also delamination because of large amount of GNP additive. As seen in (figure 3(c)) agglomeration and also delamination occurred because of large amount of GNP additive.
In the present work, we used Neural Network Toolbox of MATLAB 2016b. We have used a back-propagation (error-correction) algorithm which is a powerful learning algorithm. According to the learning algorithm, in order to reduce error, synaptic weights are changed and neural network produce new results in this way. This will be repeated until the desired result is achieved. Back-propagation algorithm is a powerful tool when the neural network has hidden layers.

The fundamental idea behind the back-propagation algorithm is to propagate errors from hidden layers to the input layers during the learning process. Back-propagation is necessary since neurons in the hidden layer
have no training target value unlike output layer so they must be trained based on errors from previous layers. When the errors are propagated backward through the nodes, synaptic weights are changed. Training happens until the errors in the weights are adequately small to be accepted \[45\].

In the \(n\)th iteration of training, if the output value of \(j\)th neuron is defined as \(y_j\) and target output from this neuron is defined as \(d_j\), error signal can be defined as follows \[36\]:

\[
e_{j}(n) = d_j(n) - y_j(n).
\]  

(2.11)

The algorithm can be written as follows \[46\]:

- Initialize the weights \(w\) from the input layer to the hidden layer and weights \(v\) from the hidden layer to the output layer. Choose the learning parameter (lies between 0 and 1) and error \(E_{\text{max}}\). Initially error is taken as 0.
- Train the network.
- Compute the error value, \(E = \frac{1}{2}(d_j - y_j)^2 + E_{\text{max}}\)
- Compute the error signal terms of the output layer and the hidden layer.
- Compute components of error gradient vectors.
- Check the weights if they are properly modified.
If $E = E_{\text{max}}$ terminate the training session. If not, go to step 2 with $E \rightarrow 0$ and initiate a new training.

For further details of this algorithm, see [43]. In the present work, the hyperbolic tangent sigmoid function (tansig) (equation (2.7)) and the linear transfer function (purelin) were used as the activation transfer functions, Levenberg–Marquardt (LM) algorithm was used as the learning rule, and the mean square error (MSE) was used as the performance function. Figure 4 shows the architecture of neural network used in this work.

There are three neurons in the input layer (density, load, reinforcements), single hidden layer with five neurons and one output neuron was modelled to predict the wear rate of the samples. There is no a for determining the number of neurons in the hidden layer. We have used an approximation given by Wong [47] as

$$n \ (\text{Number of input neurons}) \rightarrow 2n \ (\text{Number of hidden neurons}) \quad (2.12)$$

5. Results and discussions

The constructed 3-6-1 neural network model was trained and tested using the data set from table 2.

Input and output variable of each neuron in the layers must be numeric. In principle, each parameter in the model should contribute on an equal footing. Thus, to ensure equal contribution of model parameters, datasets...
were normalized according to equation (2.13)

\[ X_N = \frac{X - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}} \]  

(2.13)

where \(X_N\) is the normalized value of the \(X\), \(X_{\text{max}}\) is the maximum values of \(X\), and \(X_{\text{min}}\) is the minimum values of \(X\).

As a result of this procedure, each parameter takes a value in the interval (0,1). The training performance of this ANN model is shown in figure 5.

The training process was terminated after 7 iterations. When the number of iterations reaches its termination criterion, a mean square error (MSE) value was obtained as 0.000 000 047 708. Randomly selected 80% of the experimental data have been used for training the artificial neural network, 10% for validating and 10% for testing.

In order to test the generalization and prediction performance of the neural network, the experimental values were compared to the predicted values of ANN. Thus, a linear regression between the neural network output and experimental data is shown in figure 6.

The overall R value for all samples is 0.941 49, which shows good correlation between experimental data and total neural network response. This is an indication of good agreement between the experimental data and neural network prediction. This agreement can be also seen in figures 7(a) and (b).

Figure 7(a), infer that the wear rate declines as the GNPs reinforcement wt% rises up to 0.15 wt% additive. It is seen that 0.15 wt% GNPs and 3 wt% Si3N4 additives in the composites gave the best result compared to the pure Ti in the wear test. When GNPs reinforcement ratio increased, wear rates are increased because GNPs have agglomeration tendency partially in the composite. The inhomogeneous and locally dispersion of the GNPs led to more porous structure in composites. Therefore, the abrasive disc interact the large pure Ti zone and porous surface which causes to the deterioration of the wear properties. Figure 7(b) supports this conclusion in framework of ANN.

Figure 8 shows both of experimental and ANN results. It can be observed in the figure 8 that predicted values of the neural network follows the same trend as the experimental data. This is another achievement of the neural network of this study.

6. Conclusion

In this study, we have employed artificial neural network (ANN) method to predict wear properties of titanium hybrid composites. Titanium (Ti) was used as a matrix materials and Graphene nano-platelets (GNPs)-Si3N4 were used as a reinforcement materials in hybrid composites.

Titanium hybrid composites which we worked on were produced by PM method because it is more effective and economic for production of composites compared to other well known methods in classical way.

An ANN model for predicting the wear rate values of the composite was constructed. It has been shown that the predicted results are in good agreement with the experimental data. This implies that the wear rate can be predicted by framework of ANN with a good accuracy. It is also verified that the neural network model is reliable and predicted outputs can give an idea for developing and manufacturing new wear resistant materials.
One of the advantages of using ANN is to shorten working time and examine real physical and engineering systems in a cost effective way. The other advantage is required number of model parameters is far less than any other solution technique and therefore, compact solution models are obtained, with very low demand on memory space [48].

The results show that the predicted data maintained by ANN framework are in good agreement compared to the experimental results. A well-trained ANN system can be very helpful for estimating physical and mechanical properties of engineering systems.

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