

Article

Formulation of the Effect of Different Alloying Elements on the Tensile Strength of the *in situ* Al-Mg₂Si Composites

Halil Ibrahim Kurt * and Murat Oduncuoglu

Technical Sciences, University of Gaziantep, 27310 Gaziantep, Turkey;

E-Mail: oduncuoglu@gmail.com

* Author to whom correspondence should be addressed; E-Mail: hiakurt@gmail.com;

Tel.: +90-342-317-1700; Fax: +90-342-360-1170.

Academic Editor: Hugo F. Lopez

Received: 25 December 2014 / Accepted: 5 March 2015 / Published: 11 March 2015

Abstract: In this paper, the effect of different alloying elements on the ultimate tensile strength of Al-Mg₂Si composites is theoretically studied. The feed forward back propagation neural network with sigmoid function is used. The extensive experimental results taken from literature are modeled and mathematical formula is presented in explicit form. In addition, it is observed that magnesium and copper have a stronger effect on the ultimate tensile strength of Al-Mg₂Si composites comparison to other alloying elements. The proposed model shows good agreement with test results and can be used to find the ultimate tensile strength of Al-Mg₂Si composites.

Keywords: Al-Mg₂Si; composites; metal matrix composites; modeling

1. Introduction

In the production of composite materials, aluminum (Al), magnesium (Mg), titanium (Ti) and nickel (Ni) alloys are commonly used as metal matrix. Among the materials, Al and its alloys are the most commonly used matrix material in the production of metal matrix composites (MMCs). The composites are manufactured with the diffusion bonding, power metallurgy and casting (also known as liquid metal infiltration) processes [1]. MMCs are widely used in various industries, especially in the automotive, energy and aerospace applications, as they have excellent mechanical properties. The need to reduce emissions while enhancing performance has driven manufacturers to use more Al in industry.

This effort has been accompanied by the development of new Al alloys specifically tailored for these applications.

Al matrix composites (AMCs) reinforced by ceramic particles are prepared by *in situ* and *ex situ* methods. In the former method, the reinforce phase is synthesized internally in the matrix during the composite fabrication. In the latter method, the reinforce phase is synthesized externally and then added into the matrix during composite fabrication. The composites fabricated by these methods have important advantages such as good corrosion, high wear resistance, low cost, greater strength, compared to unreinforced materials [2,3]. Composites the produced by *in situ* technique exhibit the better particle wetting, even distribution of the reinforcing phase and thermodynamically stable system [4,5].

Al-Mg₂Si composites constitute a new category of superlight materials attracting significant interest for potential applications. The Mg₂Si intermetallic compound exhibits high melting point, low density, high hardness, low thermal expansion coefficient and reasonably high elastic modulus. The presence of Mg and silicon (Si) particles in the composite matrix with different alloying elements is considered to obtain the appropriate strength values and mechanical properties [6–8]. Additionally, the mechanical behaviors of the composites reinforced with particles were found to be a function of the matrix structure, addition alloying element, the volume fraction, particle size and shape of reinforcement [9].

The use of numerical modeling technique represents a new methodology in many different applications including materials science. One of the most used models is the artificial neural network (ANN), a form of artificial intelligence that has the ability to auto-analyze the relationship between multi-variable inputs without any hypothesis [10]. In many studies, the researchers reported that the ANN can be used as an efficient tool in predicting the properties of composite under given conditions and prescribed materials and the comparison of the designed NN and experimental results shows good agreement [11–15]. Expensive and time consuming tests are required for the determination of tensile properties of Al-based composites containing different additive element. The type and percent weight of alloying elements in the composition affect the ultimate tensile strength of the composite materials. Therefore, it is very important to select and add an element in different composition to obtain the maximum strength. The aim of this detailed theoretical study is to investigate the effect of different alloying elements on the tensile properties of *in situ* Al-Mg₂Si composites.

2. Experimental Section

The high cost-time for production and test is one of the most important barriers in the production new types of materials and composites. ANNs can accommodate multiple input variables to predict multiple output variables and are able to learn key information patterns within a multi information domain.

ANN is a mathematical model that performs a computational simulation of the behavior of neurons as in human brain and in nervous system. ANNs are capable of learning patterns by training with a number of known patterns. The learning ability of NNs procures an advantage in solving complex problems that are too difficult to solve with the analytical or numerical methods [16]. NN consists of the three components, namely: an activation function, weights and bias. Each neuron receives inputs, attached with a weight w_i , which shows the connection strength for that input for each connection.

Each input is multiplied by the corresponding weight of the neuron connection. Next, a bias (b_i) value is added to the summation of inputs and corresponding weights (u) according to following equation:

$$u_i = \sum_{j=1}^H w_{ij}x_j + b_i \quad (1)$$

The summation u_i is converted as the output with an activation (transfer) function, $f(u_i)$ yielding a value called the unit's "activation", as following formula:

$$O = f(u_i)O \quad (2)$$

Dataset and Processing

As the preprocessing of the data for ANN training, testing and validation of the models, each input and output variables are scaled to the range of 0 to 1 by the following the formula:

$$x_N = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (3)$$

where x_N is the normalized value of variable x , x_{\max} and x_{\min} are the maximum and minimum values of the variables, respectively. Output values resulted from ANN also in the range [0,1] and transformed to its equivalent values based on reverse method of normalization technique [3]. The unnormalized method is as:

$$x = x_N(x_{\max} - x_{\min}) + x_{\min} \quad (4)$$

The ANN is trained and implemented using fully developed feed forward back propagation with sigmoid function. Neural network toolbox in Matlab is used in training of the ANN. The back-propagation is an effective, supervised and the most popular learning method that consists of an input layer, one or more hidden layers and an output layer [17–19]. Sigmoid function is an activation function joins curvilinear, linear and constant behavior depending on the values of the input in ANN system [20,21]. In the ANN, mean square error (MSE) and mean absolute error (MAE) are used as error evaluation criteria in order to facilitate the comparisons between predicted values and desired values. MSE and MAE were calculated by the program.

3. Results and Explicit Formulation of NN Model

The aim of this study is nominal strength prediction of Al-Mg₂Si composite materials containing different alloying elements. Therefore, an extensive literature survey has been performed for available experimental results [22–31]. The experimental datasets are divided into three sets as training, validation and test dataset to avoid the over fitting problems. The datasets for training, validation and test are randomly selected from among experimental results where 40 sets are training set as shown in Table 1, 9 sets are validation and test sets as shown in Table 2.

Table 1. Training input data (wt.%).

Data Number	Mg	Si	Cu	Mn	Cr	P	Be	B	Li	Y	Na	Al
1	16.2	9.1	0.01	0.03	0.02	-	-	-	-	-	-	Rem.
2	16.2	9.1	0.01	0.03	0.02	0.1	-	-	-	-	-	Rem.
3	16.2	9.1	0.01	0.03	0.02	0.5	-	-	-	-	-	Rem.
4	16.2	9.1	0.01	0.03	0.02	3	-	-	-	-	-	Rem.
5	9.5	5.5	0.01	0.01	0.02	-	0.1	-	-	-	-	Rem.
6	9.5	5.5	0.01	0.01	0.02	-	0.5	-	-	-	-	Rem.
7	9.68	5.7	0.02	0.02	0.01	-	-	-	-	-	-	Rem.
8	9.68	5.7	0.01	0.01	0.52	-	-	-	-	-	-	Rem.
9	9.68	5.7	0.01	0.01	1.02	-	-	-	-	-	-	Rem.
10	9.68	5.7	0.01	0.01	2.02	-	-	-	-	-	-	Rem.
11	9.5	5.5	0.01	0.01	0.02	-	-	0.1	-	-	-	Rem.
12	9.5	5.5	0.01	0.01	0.02	-	-	0.5	-	-	-	Rem.
13	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
14	9.7	5.5	0.01	0.51	0.02	-	-	-	-	-	-	Rem.
15	9.7	5.5	0.01	1.01	0.02	-	-	-	-	-	-	Rem.
16	9.7	5.5	0.01	2.01	0.02	-	-	-	-	-	-	Rem.
17	9.7	5.5	0.01	3.01	0.02	-	-	-	-	-	-	Rem.
18	9.7	5.5	0.01	5.01	0.02	-	-	-	-	-	-	Rem.
19	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
20	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
21	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
22	9.7	5.5	0.01	0.01	0.02	-	-	-	0	-	-	Rem.
23	9.7	5.5	0.01	0.02	0.01	-	-	-	5.5	-	-	Rem.
24	9.74	6	0.01	0.01	0.03	-	-	-	6.12	-	-	Rem.
25	9.47	7	0.01	0.01	0.02	-	-	-	7.11	-	-	Rem.
26	9.54	11	0.01	0.02	0.03	-	-	-	1.37	-	-	Rem.
27	9.7	5.5	0.01	0.02	0.01	-	-	-	-	-	-	Rem.
28	9.7	5.5	0.01	0.01	0.02	-	-	-	-	0.1	-	Rem.
29	9.7	5.5	0.01	0.01	0.02	-	-	-	-	0.5	-	Rem.
30	9.7	5.5	0.01	0.01	0.02	-	-	-	-	1	-	Rem.
31	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
32	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	0.01	Rem.
33	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	0.05	Rem.
34	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	0.08	Rem.
35	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	0.15	Rem.
36	9.82	5.7	0.11	0.01	0.01	-	-	-	-	-	-	Rem.
37	9.82	5.7	0.31	0.01	0.02	-	-	-	-	-	-	Rem.
38	9.82	5.7	0.51	0.01	0.02	-	-	-	-	-	-	Rem.
39	9.82	5.7	1.01	0.01	0.02	-	-	-	-	-	-	Rem.
40	9.82	5.7	5.01	0.01	0.02	-	-	-	-	-	-	Rem.

The input (independent) variables are Al, Mg, Si, copper (Cu), manganese (Mn), chromium (Cr), phosphorus (P), beryllium (Be), boron (B), lithium (Li), yttrium (Y) and sodium (Na) wt.%. The output

(dependent) variable is the ultimate tensile strength (UTS) in unit of MPa. Levenberg–Marquardt (Trainlm) algorithm with back propagation is used in the training of NN.

Table 2. Validation and test input data (wt.%).

Part	Data Number	Mg	Si	Cu	Mn	Cr	P	Be	B	Li	Y	Na	Al
Validation	1	16.2	9.1	0.01	0.03	0.02	1	-	-	-	-	-	Rem.
	2	9.5	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
	3	9.68	5.7	0.01	0.01	5.02	-	-	-	-	-	-	Rem.
	4	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
	5	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
	6	9.66	6.5	0.01	0.01	0.02	-	-	-	6.45	-	-	Rem.
	7	9.52	13	0.02	0.02	0.03	-	-	-	12.7	-	-	Rem.
	8	9.7	5.5	0.01	0.01	0.02	-	-	-	-	0.3	-	Rem.
	9	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
Test	1	16.2	9.1	0.01	0.03	0.02	0.1	-	-	-	-	-	Rem.
	2	9.5	5.5	0.01	0.01	0.02	-	0.3	-	-	-	-	Rem.
	3	9.68	5.7	0.01	0.01	3.02	-	-	-	-	-	-	Rem.
	4	9.5	5.5	0.01	0.01	0.02	-	-	-	-	-	-	Rem.
	5	9.5	5.5	0.01	0.01	0.02	-	-	0.3	-	-	-	Rem.
	6	9.5	5.5	0.01	0.01	0.02	-	-	1	-	-	-	Rem.
	7	9.62	7.5	0.01	0.01	0.02	-	-	-	7.65	-	-	Rem.
	8	9.7	5.5	0.01	0.01	0.02	-	-	-	-	-	0.2	Rem.
	9	9.82	5.7	3.01	0.01	0.02	-	-	-	-	-	-	Rem.

The performance of an NN is affected by the network architecture, initial weight and learning rate. One of the most difficult tasks in NN works is the determination of the number of hidden layers and the number of neurons in per layer. There is no well-defined procedure to find the optimal settings of parameters and network architecture. The trial and error approach is used to determine the number of neurons in the hidden layer. Three different neuron numbers in one hidden layer (12, 13 and 14) are used in this study. The training data set (70%) is used to determine the weights and learning ability of the network. It is known that increasing the data used in training process of NN enhances the learning ability of NN. After the network is trained, the validation dataset is used to measure the performance and generalization ability of the network. The test dataset is used to verify the effectiveness of the network and to estimate the expected performance in the future. It is observed that the optimal NN architecture is found to be 12–12–1 NN architecture with logistic sigmoid transfer function.

The experimental results are compared with the predicted results for the performance of NN model. Figure 1 shows the correlation of NN and experimental results for training set.

In the all stages of NN work, the effects of the percent weight of alloying elements on the strength of Al-Mg₂Si composites are quantified. The prediction accuracy of NN for training set is quite satisfactory. Severe deviations between the experimental and theoretical results are observed in training of NN. These can be attributed to the sizes, volume fraction and morphology of Mg₂Si phase and other phases formed in the matrix and variation in experimental conditions. It is known that the

various geometric shapes of Mg_2Si crystals and the formation and morphology of intermetallic phases have an important effect on the strength of Al- Mg_2Si composites [32].

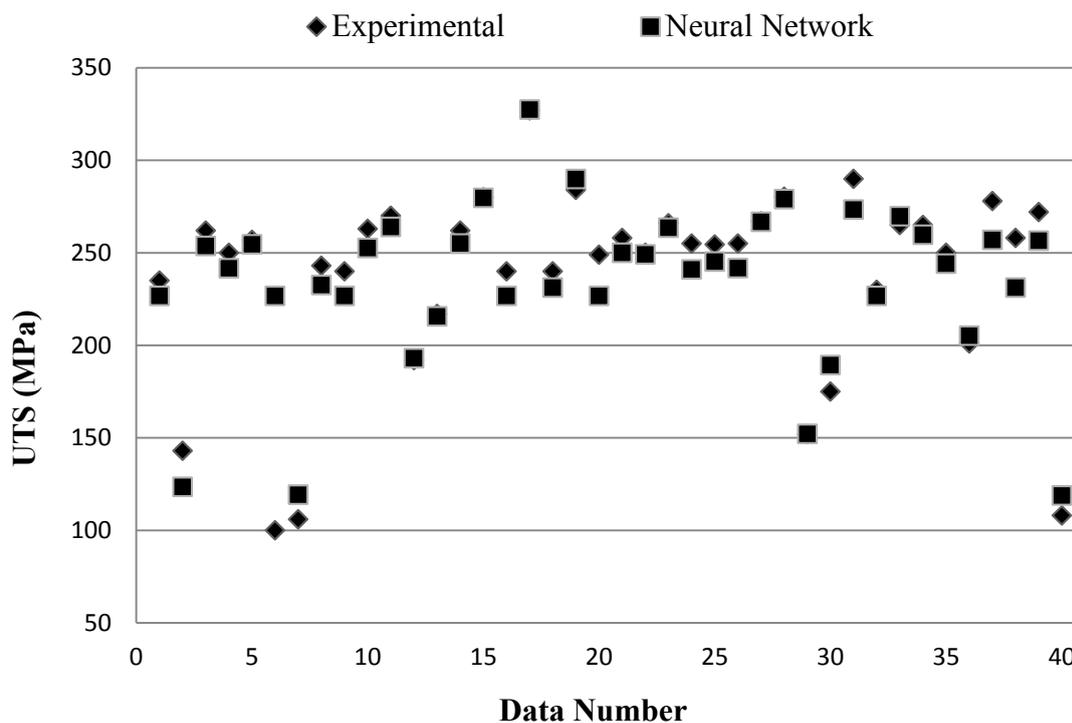


Figure 1. Correlation of NN and experimental results for training set.

The correlation of NN and experimental results for validation and test sets are shown in Figure 2a,b, respectively. After the network is trained, the validation data (Figure 2a) are used to check that the model behaves correctly when presented with previously unseen data. The validation (15%) and test (15%) data sets are randomly selected by program from among 58 experimental data. It is not interfered to the program in the selection stage of the data sets. It is clearly seen from Figure 2 that the experimental and predicted values developed from ANN for UTS are very close to each other and it can also be seen a few minor deviations. The predictability ratio of proposed NN increases from training to test set.

The statistical parameters of training, validation and test datasets of the NN model is given in Table 3. In the train set, the observed correlation coefficient (R) is 0.899, which means that the performance of trained network model is acceptable. The model is verified against the cases in the test dataset, which are independent of the cases in the train dataset. The predicted results are plotted versus the experimental results. As shown in Table 3, the correlation coefficients of validation and test sets are 0.932 and 0.951, indicating that the network can predict the UTS of Al- Mg_2Si composite materials with high accuracy and reliability. It can be said that the using of all the alloying elements with the different weight ratio in the training stage of NN is contributed to the increasing of R values of the validation and test sets.

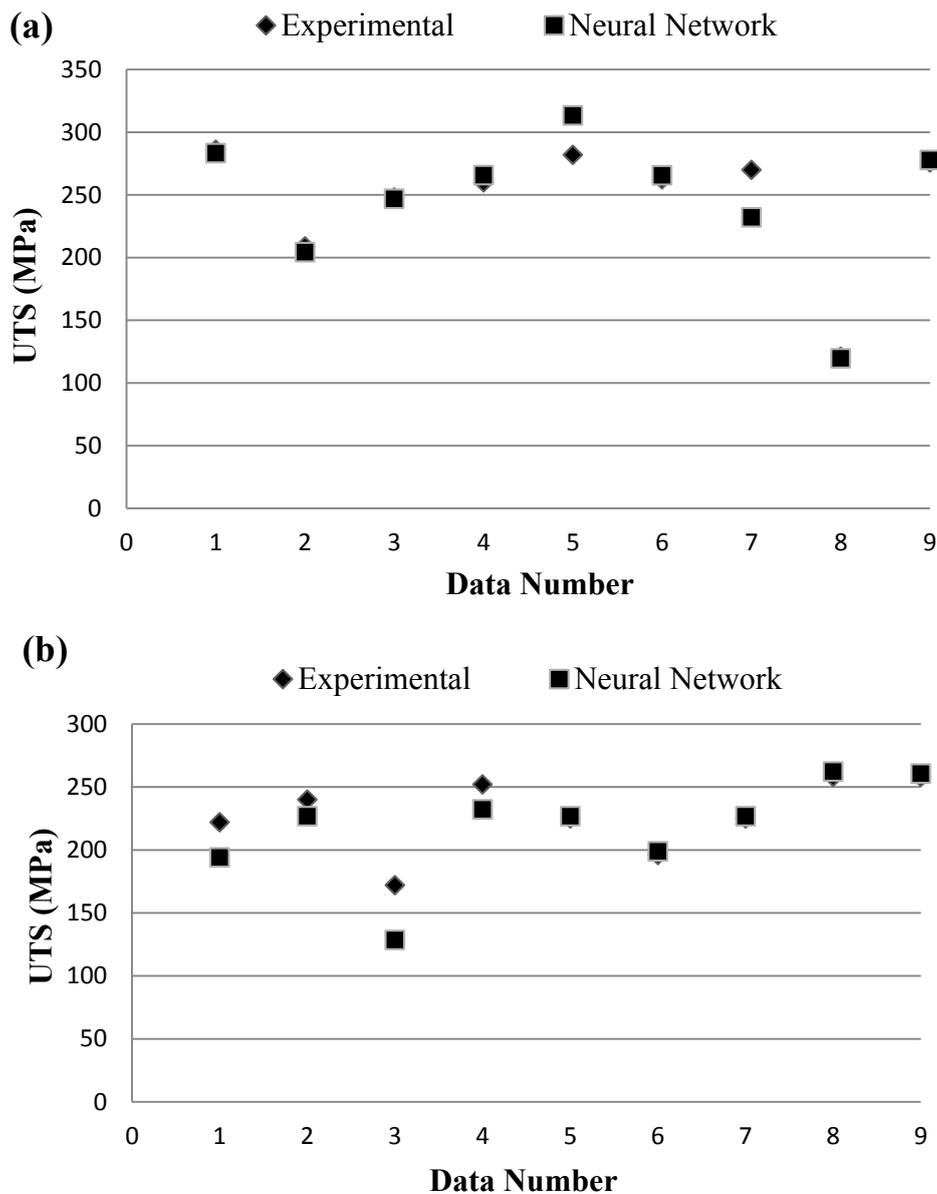


Figure 2. Correlation of neural network (NN) and experimental results for (a) validation and (b) test sets.

Table 3. Statistical parameters of train, validation and test sets.

Part	R	MSE	MAE
Train set	0.899	1.005	5.123
Validation set	0.932	0.706	5.765
Test set	0.951	0.537	4.385

As mentioned before, the effects of the percent weight of alloying elements on the strength of Al-Mg₂Si are considered. The change in UTS values are probably due to the sizes, volume fraction and morphology of the phases and it needs extensive studies. Nevertheless, R values of training, validation and test sets indicate that the learning ability of NN is well enough and the proposed NN model has high accuracy.

MSE and MAE are used to fix the performance of the proposed NN in prediction technique. MSE is 1.005% for training set, 0.706% for validation set and 0.537% for test set. If the MSE reaches zero, the performance of model is regarded as the excellent [13]. MAE is 5.123% for training set, 5.765% for validation set and 4.385% for test set. It is clear that the level of error decreases from training set to test set. These error criteria show that the main source of prediction error is the “noise” in the experimental data. These levels of error can be accepted and considered to be satisfactory. It can be said that the UTS of Al-Mg₂Si composites can be predicted by ANN model with 95.1% accuracy and the presented NN model is in good agreement with the experimental data and all errors are within acceptable ranges. The sensitivity of input vectors on UTS of Al-Mg₂Si composites is given in Figure 3.

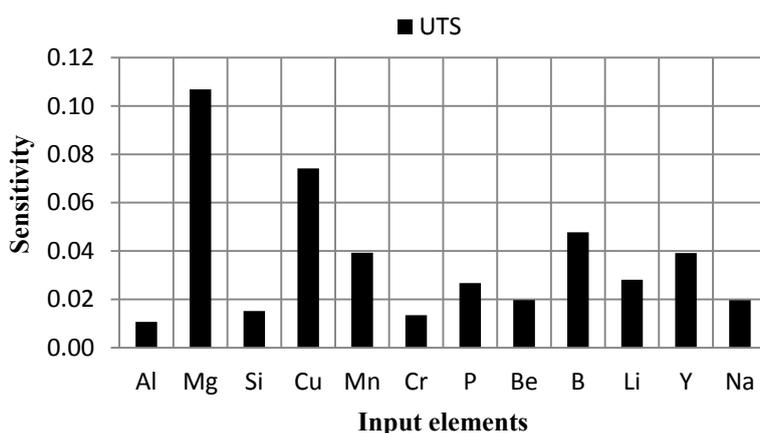


Figure 3. The sensitivity of input vectors.

The mechanical property of the *in situ* composites has a great relationship with the size and morphology of the Mg₂Si phases [33]. It is seen that Mg has more impact on UTS of Al-Mg₂Si composites than the other alloying elements. Any change in Mg and Cu levels will have significant effect the UTS.

The main focus is to obtain the explicit formulation of UTS for Al-Mg₂Si composites as a function of addition alloying elements. The proposed equation below is obtained using a developed macro in Matlab program. It should be noted that the proposed explicit formulation is valid for the ranges of training set.

$$Y = 227 \times \left(\frac{1}{1 + e^{-w}} \right) + 100 \tag{5}$$

where *Y* is the ultimate tensile strength and *w* is

$$w = (-2.92) * \left(\frac{1}{1 + e^{-u1}} \right) + (0.19) * \left(\frac{1}{1 + e^{-u2}} \right) + (-2.66) * \left(\frac{1}{1 + e^{-u3}} \right) + (1.18) * \left(\frac{1}{1 + e^{-u4}} \right) + (0.66) * \left(\frac{1}{1 + e^{-u5}} \right) + (-0.47) * \left(\frac{1}{1 + e^{-u6}} \right) + (1.30) * \left(\frac{1}{1 + e^{-u7}} \right) + (0.28) * \left(\frac{1}{1 + e^{-u8}} \right) + (2.29) * \left(\frac{1}{1 + e^{-u9}} \right) + (-4.70) * \left(\frac{1}{1 + e^{-u10}} \right) + (0.88) * \left(\frac{1}{1 + e^{-u11}} \right) + (-1.01) * \left(\frac{1}{1 + e^{-u12}} \right) + 0.99$$

where

$$u_1 = (-0.81) * K_1 + (1.70) * K_2 + (1.24) * K_3 + (-1.86) * K_4 + (0.37) * K_5 + (0.50) * K_6 + (-0.21) * K_7 + (-0.92) * K_8 + (-3.10) * K_9 + (1.83) * K_{10} + (-0.85) * K_{11} + (0.20) * K_2 + (0.47)$$

$$u_2 = (0.60) * K_1 + (-1.29) * K_2 + (-0.33) * K_3 + (1.63) * K_4 + (0.07) * K_5 + (0.62) * K_6 + (0.75) * K_7 + (0.78) * K_8 + (0.80) * K_9 + (0.07) * K_{10} + (0.51) * K_{11} + (0.58) * K_2 + (0.06)$$

$$u_3 = (0.19) * K_1 + (-0.24) * K_2 + (-2.11) * K_3 + (-0.78) * K_4 + (-0.09) * K_5 + (-0.35) * K_6 + (-0.66) * K_7 + (0.65) * K_8 + (0.57) * K_9 + (-0.08) * K_{10} + (0.88) * K_{11} + (0.58) * K_2 + (-0.93)$$

$$u_4 = (0.57) * K_1 + (-1.63) * K_2 + (-0.88) * K_3 + (1.56) * K_4 + (0.31) * K_5 + (0.02) * K_6 + (0.43) * K_7 + (0.75) * K_8 + (1.57) * K_9 + (-0.79) * K_{10} + (0.09) * K_{11} + (-1.16) * K_2 + (0.51)$$

$$u_5 = (0.30) * K_1 + (-1.08) * K_2 + (-0.87) * K_3 + (1.94) * K_4 + (0.89) * K_5 + (0.44) * K_6 + (0.70) * K_7 + (0.82) * K_8 + (1.92) * K_9 + (-0.03) * K_{10} + (0.73) * K_{11} + (0.89) * K_2 + (0.43)$$

$$u_6 = (-0.10) * K_1 + (0.47) * K_2 + (0.24) * K_3 + (-0.39) * K_4 + (0.25) * K_5 + (-0.06) * K_6 + (0.09) * K_7 + (-0.51) * K_8 + (0.22) * K_9 + (0.11) * K_{10} + (0.04) * K_{11} + (0.12) * K_2 + (0.36)$$

$$u_7 = (0.56) * K_1 + (-0.33) * K_2 + (-0.82) * K_3 + (0.19) * K_4 + (-0.69) * K_5 + (0.07) * K_6 + (0.65) * K_7 + (0.33) * K_8 + (0.42) * K_9 + (0.70) * K_{10} + (1.08) * K_{11} + (0.35) * K_2 + (0.82)$$

$$u_8 = (0.49) * K_1 + (-1.50) * K_2 + (-0.70) * K_3 + (0.90) * K_4 + (0.57) * K_5 + (0.17) * K_6 + (0.20) * K_7 + (0.13) * K_8 + (0.91) * K_9 + (0.03) * K_{10} + (0.69) * K_{11} + (0.82) * K_2 + (0.53)$$

$$u_9 = (0.37) * K_1 + (-0.79) * K_2 + (-0.10) * K_3 + (0.88) * K_4 + (-0.08) * K_5 + (0.03) * K_6 + (0.42) * K_7 + (-0.06) * K_8 + (-0.74) * K_9 + (0.26) * K_{10} + (-0.65) * K_{11} + (-0.36) * K_2 + (0.10)$$

$$u_{10} = (1.21) * K_1 + (1.26) * K_2 + (-1.75) * K_3 + (-1.79) * K_4 + (-3.59) * K_5 + (-1.40) * K_6 + (-0.44) * K_7 + (-0.89) * K_8 + (-0.68) * K_9 + (0.22) * K_{10} + (-3.15) * K_{11} + (-2.48) * K_2 + (-1.46)$$

$$u_{11} = (0.23) * K_1 + (-0.20) * K_2 + (-0.47) * K_3 + (0.18) * K_4 + (-0.09) * K_5 + (0.07) * K_6 + (0.38) * K_7 + (-0.37) * K_8 + (-0.68) * K_9 + (0.70) * K_{10} + (-0.22) * K_{11} + (-0.07) * K_2 + (0.22)$$

$$u_{12} = (0.68) * K_1 + (-0.33) * K_2 + (-0.41) * K_3 + (1.32) * K_4 + (0.32) * K_5 + (0.41) * K_6 + (0.20) * K_7 + (0.74) * K_8 + (0.49) * K_9 + (-0.84) * K_{10} + (0.27) * K_{11} + (0.53) * K_2 + (0.04)$$

where $K_1, K_2, K_3, K_4, K_5, K_6, K_7, K_8, K_9, K_{10}, K_{11}$ and K_{12} are normalized input data of Al, Mg, Si, Fe, Cu, Mn, Cr, Ti, Ni, Zn, P, Zr, Be, B, Li, Y and Na.

The training data set contains the weight percentage of all alloying elements and is used to determine the best set of neural network weights. Thus, the proposed equation can be used for determining the effects of all alloying elements on the strength of Al-Mg₂Si composites. It is observed that the strength of Al-9.5Mg-5.5Si-0.01Cu-0.01Mn-0.02Cr alloy used in test set with 3 wt.% Cu increased from 252 to 317 ± 12 MPa using the derived formula. The multiple minor alloying elements (0.02P + 0.15Be + 0.2B + 0.2Y + 0.03Na wt.%) is theoretically added into

Al-16.2Mg-9.1Si-0.01Cu-0.03Mn-0.02Cr alloy. The strength of the alloy is increased from 108 to 189 ± 9 MPa. The main reason for this improvement can be attributed to the precipitation of more primary complex particles [34].

4. Conclusions

This work proposes an approach for ultimate tensile strength in prediction of Al-Mg₂Si composites containing different alloying elements. The back propagation NNs are used for the training process and the proposed NN model shows good agreement with experimental results. The results also demonstrate that all the data sets have quite high correlation and accuracy. Therefore, the mathematical function is derived in explicit form by using ANN. The outcomes of the study are very promising in general. The mean absolute error for predicted values does not exceed 5.8%. The sensitivity analysis of the model demonstrated that the addition of Mg has greater effect than the other elements on the UTS of Al-M₂Si composites. Hence it is concluded that considerable saving in terms of cost and time could be obtained by using the model and ANN is a successful analytical tool provided it is properly used.

Author Contributions

These authors contributed equally to this work. Kurt and Oduncuoglu analyzed and interpreted the data and prepared the manuscript. All authors discussed the conclusions and reviewed the manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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