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Prediction of Tensile Property of Hydrogenated Ti600 Titanium Alloy Using Artificial Neural Network

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An artificial neural network (ANN) model has been developed to analyze and predict the correlation between tensile property and hydrogenation temperature and hydrogen content of hydrogenated Ti600 titanium alloy. The input parameters of the neural network model are hydrogenation temperature and hydrogen content. The output is ultimate tensile strength. The accuracy of ANN model was tested by the testing data samples. The prediction capability of ANN model was compared with the multiple linear regression approach and response surface method. The combined influence of inputs on the tensile property is also simulated using ANN model. It is found that excellent performance of the ANN model was achieved, and the results showed good agreement with experimental data. Moreover, the developed ANN model can be used as a tool to control the tensile property of titanium alloys.

Keywords artificial neural network, hydrogenation, tensile property, Ti600 alloy

1. Introduction

Thermohydrogen processing (THP) is an attractive approach which correctly uses hydrogen as a temporary alloying element to enhance working qualities and modify microstructure to improve mechanical properties (Ref 1-3). After hydrogenation of titanium alloy, the β transus temperature decreases and the proportion of β phase increases. Because the β phase with body-centered cubic (BCC) structure can be easily deformed at high temperature, the addition of hydrogen reduces the flow stress of α and α + β titanium alloys in α single-phase and α + β two-phase regions. There have been some reports on hydrogenation of titanium alloys to improve the hot workability. D. B. Shan (Ref 4) discussed the strengthening effect of hydrogen on the β phase and the softening effect of hydrogen on the α phase, and some optimizations of hydrogen content and deformation temperature were developed. Y. Zhang (Ref 5) found that the minimum of peak compression flow stresses at 900-1000 °C was obtained when the 0.2 wt.% hydrogen was added into the Ti-25Al-10Nb-3V-1Mo alloy, which corresponds to decreasing the deformation temperature by about 50 °C. Therefore, the use of hydrogen as a temporary alloying element is always added into titanium alloys to improve the workability during hot deformation processing.

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Ti600 alloy designed and developed by Northwest Institute for Nonferrous Metal Research is a new type of near-α titanium alloy. With the rapid development of aviation engines, higher service temperature has been increasingly demanded (Ref 6). Ti600 titanium alloy can be used for aviation engine serviced at 600 °C because of its excellent creep performance, good ultimate strength, and superior fatigue resistance. Some research groups have done a lot of helpful work about this alloy with regard to the aspects of kinetics of hydrogen absorption (Ref 7) and hot deformation behavior at elevated temperature (Ref 8). However, due to the narrow processing window and poor workability, it is difficult to control the deformation processing of Ti600 alloy, thus how to improve the hot deformation workability of this alloy has become an international scholars' research focus. It is generally found that the addition of hydrogen can remarkably decrease the flow stress of the alloy, which implies that the deformation temperature can be decreased. As the THP greatly depends on the hydrogenation temperature and hydrogen content, it is very important to understand the influence of these two factors on the tensile property of alloys.

Recently, the artificial neural network (ANN) technique has been developed to become one of the fundamentally powerful modeling tools in comparison to the statistical or numerical methods. Based on a nonlinear statistical approach, it is suitable for simulations of correlations which are hard to describe by conventional methods. It has been applied successfully in many areas of engineering and has produced promising preliminary results in the fields of material modeling and processing (Ref 9-13). Hence, in this study, the prediction of tensile property of hydrogenated Ti600 alloy has been modeled using ANN, in which network training was accomplished with the neural network toolbox written in MATLAB environment. The back-propagation (BP) learning algorithm was used in the training stage. Details of ANN used to study the influence of hydrogenation temperature and hydrogen content on the tensile property of hydrogenated Ti600 alloy are presented in the following sections.

2. Experimental Procedures

The received Ti600 alloy provided by Northwest Institute for Nonferrous Metal Research is in form of sheet with a thickness of 2 mm. The nominal composition is 6Al-2.8Sn-4Zr-0.5Mo-0.4Si-0.1Y (wt.%). The thermohydrogen treatment was conducted in a stainless steel tube, mounted in a tube-type furnace. All the specimens were hydrogenated at 600, 650, 700, and 750 °C for 1 h followed by air cooled to room temperature. Specimens with various hydrogen contents were obtained by controlling the varied charging time, while the flow rate of hydrogen was fixed to 1 L min^{-1}. The actual hydrogen content in specimen was determined by weighing the specimens before and after hydrogenation using an analytic balance providing an accuracy of 10^{-5} g. In this study, specimens with hydrogen content of 0.081, 0.161, 0.319, 0.393, and 0.507 wt.% were obtained. Tensile test was carried out on Zwick/Z150 universal testing machine in the temperature range from 600 to 750 °C with 50 °C interval at an initial strain rate of 2 s^{-1}.

3. Development of ANN Model

3.1 The Principle of the ANN Model

An ANN attempts to simulate the biological structure of the human brain and nervous system. It gathers information through a learning process from the outside environment. The inter-neuron connection strengths known as synaptic weights are used to store knowledge (Ref 14). This adaptive learning ability of neural networks gives an advantage in solving complex problems whose analytic or numerical solutions are difficult to obtain.

A typical neural network consists of a sequence of layers with full connections between successive layers. There are usually two layers: an input layer and an output layer. In the input layer, data are presented to the neural network, while the output layer holds the response of the network to the input. The layer between the input and the output layers is the hidden layer, which enable these networks to represent and compute complicated associations between inputs and outputs. The three layers consist of a number of small individual interconnected processing units, usually called as neurons. Theses neurons interact with each other via weighted connections.

Recently, the most popular and effective supervised learning algorithm known in the field of neural networks is the BP neural network (Ref 15, 16). Figure 1 shows an example of the structure of a BP neural network with one input, one hidden and one output layer. It can be seen from Fig. 1 that the input patterns of each node are provided from input layer first. Then this signal is converted at each node and transferred to the hidden layer. Finally, the signal generates outputs in the output layer. The output values are compared to the target values, if there is a difference, the connection weights are adjusted in such a direction that the error is decreased. This adjustment is back propagated from the upper layers to the lower layers, which results in the adjustment of the connection weights in the lower layers (Ref 17). In the hidden layers and output layer, each node first acts as a summing junction which combines and modifies the inputs from the previous layer using Eq 1. The each node transfers the summation to the output of the node through a sigmoid function (Eq 2).

$$y_i = \sum_j x_j w_{ij} + b_i \quad \text{(Eq 1)}$$

$$z_i = \frac{1}{1 + \exp(-y_i)} \quad \text{(Eq 2)}$$

where y_i is the total inputs of the ith node in the layer, w_{ij} is the weight from the jth to the ith neuron, b_i is the threshold of the ith neuron, and x_j is one of the inputs of the ith neuron, z_i is the output of the ith neuron. The equation to update the weights in momentum learning is (Ref 18):

$$w_{ij}(n+1) = w_{ij}(n) + \eta\delta_i x_j + \alpha\Delta w_{ij}(n) \quad \text{(Eq 3)}$$

where w_{ij} is the weight between nodes i and j at iteration n is discrete time, η is the learning rate, δ_i is the difference between actual and predicted values, α is momentum value and is set to a value between 0.1 to 0.9.

3.2 Modeling and Training by BP Neural Network

The procedure of ANN modeling is usually within the following contexts: (a) collection and pre-processing of data,

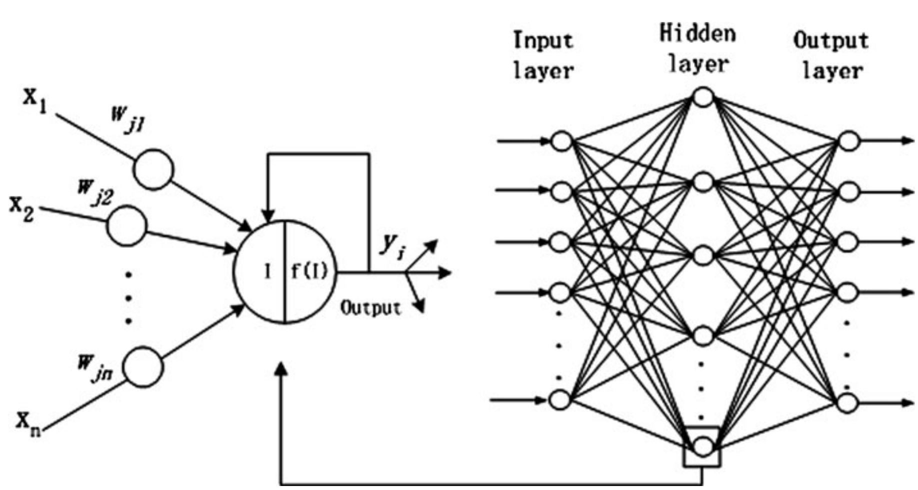

Fig. 1 The model of processing unit and architecture of neural network

(b) training of neural networks, (c) testing of the trained neural networks, and (d) using the trained neural networks for simulation and prediction (Ref 19). These steps were used in the developing of the model presented in this article.

The experimental data set was divided into the training data at 600, 650 and 700 °C, and the testing data at 750 °C. Before training the network, all the data sets must be normalized for the ANN learning to prevent a specific factor from dominating the learning. In general, normalization gives a value between 0 and 1. However, in this study, it is recommended that the data be normalized between slightly offset values such as 0.1 and 0.9 to prevent the generation of 0 and 1 as (Ref 20):

$$X' = 0.8\frac{X - X_{\min}}{X_{\max} - X_{\min}} + 0.1 \quad \text{(Eq 4)}$$

where X' is the normalized value of X, and $X_{\max}$ and $X_{\min}$ are the maximum and minimum values of X, respectively. After the neural network was trained, tested, and simulated, it is necessary for the simulating data to be unnormalized corresponded with normalization. The unnormalized method is as:

$$X = \frac{(X' - 0.1)(X_{\max} - X_{\min})}{0.8} + X_{\min} \quad \text{(Eq 5)}$$

The number of neurons in the input and output layers are usually determined based on the number of parameters affecting the process and the complexity of the relationships existing between them. In this study, the input parameters consist of two input nodes representing the hydrogenation temperature and hydrogen content, while the output parameters are ultimate tensile strength.

In order to decide the optimum structure of neural network, the trial and error method was used to obtain the number of neurons in the hidden layer so that the error between the desired and the estimated outputs was minimized. The minimum mean square errors (MSEs) of computations were used as the performance criteria. MSE was computed according to the following equation:

$$\text{MSE} = \left(\frac{1}{N}\sum_{i=1}^{N}|t_i - \hat{t}_i|\right)^2 \quad \text{(Eq 6)}$$

where t is the measured value, y is the predicted value, and N is the number of the sample. If the MSE reaches 0, the performance of model is regarded as the excellent. The effect of the number of neurons in the hidden layer on the network performance is shown in Fig. 2. It can be observed that the MSE reaches minimum with 10 neurons in the hidden layer, indicating the performance of network is best when the number of hidden layer neurons is 10.

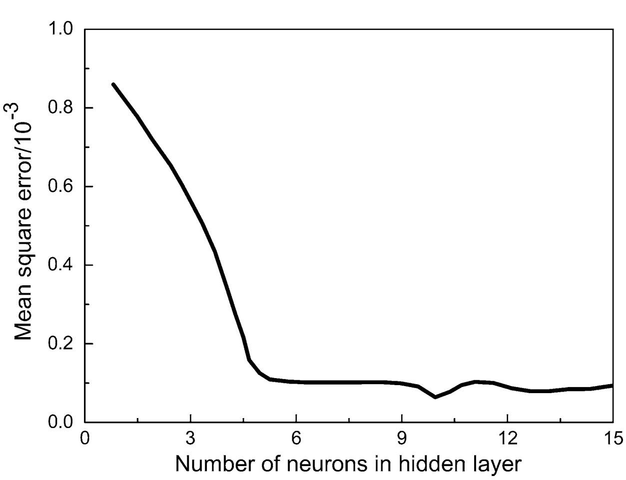

Fig. 2 Influence of hidden nodes on the network performance

The training process was carried out with the training data set, in which the corresponding outputs are known, the weight connections were adjusted until the predicted output agrees with the experimental values, then the connection weights are stored in form of text file to further be used for testing the developed neural network. After several adjustments to the network parameters, a three-layer BP neural network with the structure of 2-10-1 shows the best performance. To ensure that a network is not over-fitted, training should be stopped as soon as the MSE with respect to the test set reaches a minimum. The simulation results can be obtained by testing the network after the training completed.

4. Results and Discussions

4.1 Experimental Results

Ultimate tensile property data of hydrogenated Ti600 alloy listed in Table 1 were obtained from testing machine after high-temperature tensile tests. In order to present the relationship between hydrogen content and tensile property more obviously, the relation curves for specimens with various hydrogen contents in the temperature range of 600 to 750 °C were plotted in the Fig. 3. As can be seen from Fig. 3, the ultimate tensile strength decreased with the increasing hydrogen content, which is consistent with literature (Ref 21). Although much

Table 1 Experimental data of high temperature tensile test of hydrogenated Ti600 alloy

Hydrogenation temperature, °C	Hydrogen content, wt.%	Ultimate tensile strength, MPa
600	0	640.0
	0.081	605.0
	0.161	595.0
	0.319	550.0
	0.393	520.0
	0.507	485.0
650	0	585.0
	0.081	555.0
	0.161	515.0
	0.319	440.0
	0.393	415.0
	0.507	395.0
700	0	495.0
	0.081	455.0
	0.161	450.0
	0.319	350.0
	0.393	335.0
	0.507	295.0
750	0	420.0
	0.081	365.0
	0.161	285.0
	0.319	290.0
	0.393	210.0
	0.507	200.0

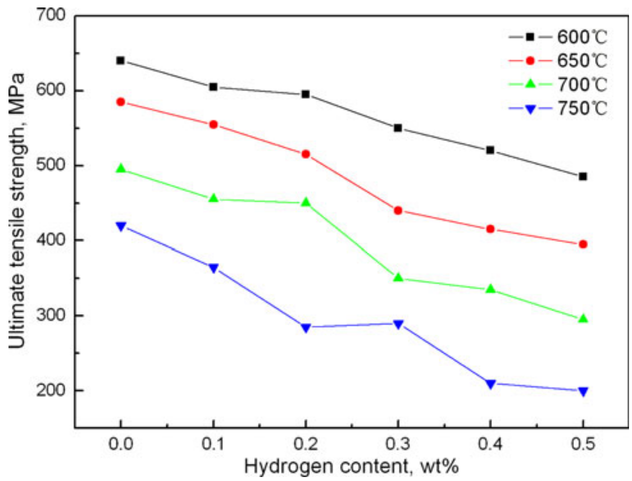

Fig. 3 Relationship between hydrogen content and tensile property of hydrogenated Ti600 alloy

attention with regard to the effect of hydrogen on the deformation mechanism of high-temperature titanium alloys has been drawn (Ref 22-24), the accordant conclusion is still lack of in deep study. Currently, it has been generally suggested that the decrease of ultimate tensile strength is related to the increase of β phase. Because hydrogen is β-stabilizing element, it destabilizes the hexagonal close packed (hcp) α phase and stabilize the softer BCC β phase in titanium alloys, the volume fraction of β phase increases with the addition of hydrogen (Ref 25).

4.2 The Prediction of ANN

Having trained the network successfully with data at 600, 650, and 700 °C, the next procedure is to test the network model for the purpose to check its performance and to determine whether the predicted results agree with the actual results. To test the generalization performance of the trained network model in testing and validating processes, the predicted values resulted from ANN were compared to the experimental values (Fig. 4). The performance of the network model for tensile property prediction was evaluated in the form of correlation coefficient between the experimental data and the corresponding predicted result. In Fig. 4(a), the corresponding correlation coefficient (R) is 0.998, which means that the performance of trained network model is very good. Subsequently, the ultimate tensile strength values predicted by ANN using validating dataset (at 750 °C) were compared with experimental values. As shown in Fig. 4(b), the correlation coefficient is 0.974, indicating that the network can predict the ultimate tensile strength of hydrogenated Ti600 alloy with high accuracy and reliability. Furthermore, on the basis of the training and testing data sets, the results obtained by network model and the absolute/relative error of predicted data compared to the experimental values are calculated, and the relative error results are presented graphically as error bars in Fig. 5. It can be observed that the average of absolute error is −1.87 MPa and the maximum value of absolute error is 12.7 MPa. The relative error demonstrates that for more than 90% testing and validating dataset, the relative error does not exceed 5%. This signifies that main source of prediction error is the noise in the experimental data and cannot be wholly

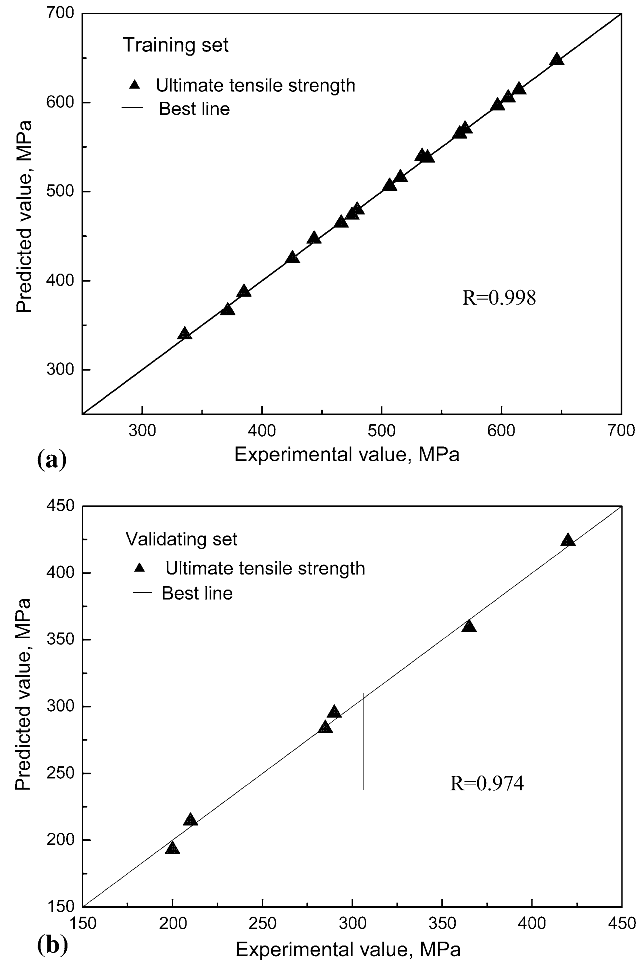

Fig. 4 Experimental vs. predicted values for studied properties (a) training dataset and (b) validating dataset

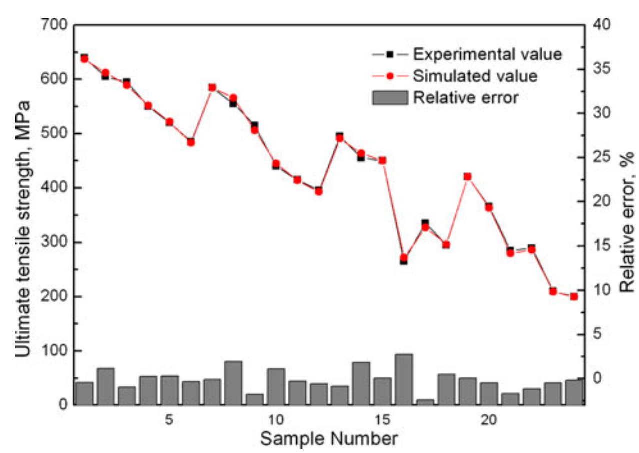

Fig. 5 Experimental results vs. ANN results of tensile property for hydrogenated Ti600 alloy

attributed to the predict ability of the neural network model. In order to verify the prediction capability of ANN model further, the multiple linear regression (MLR) approach and response surface method (RSM) were used to modeling the relationship between ultimate tensile strength and hydrogen content as well as hydrogenation temperature based on the data sets at 750 °C,

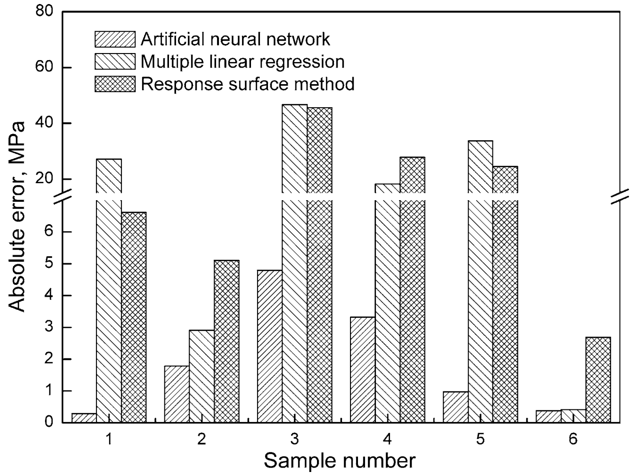

Fig. 6 Comparison of error of predicted value from ANN to calculated value from MLR and RSM at 750 °C

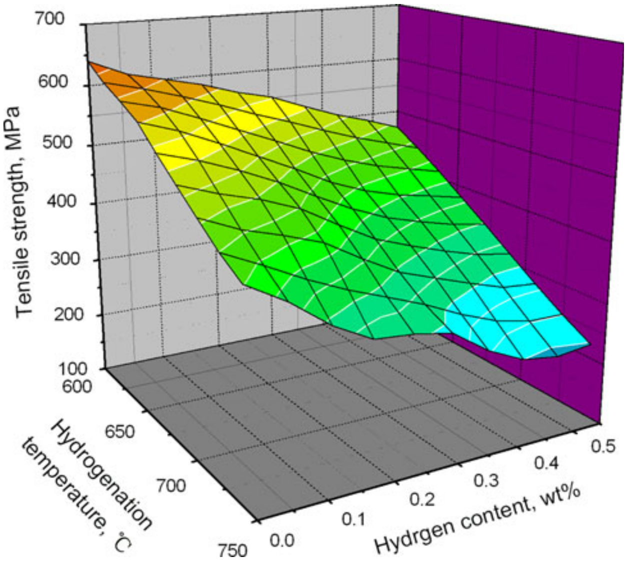

Fig. 7 Combined influence of hydrogenation temperature and hydrogen content on ultimate tensile strength of hydrogenated Ti600 alloy

respectively. The mathematical expressions are shown as Eq 7 and 8.

$$Y = -1.8X_1 - 379.5X_2 + 1742.8 \quad \text{(Eq 7)}$$

$$Y = 945.89 + 0.49X_1 - 134.93X_2 - 0.00016X_1^2 + 253.92X_2^2 - 0.56X_1X_2 \quad \text{(Eq 8)}$$

where Y is ultimate tensile strength, X_1 is hydrogenation temperature, and X_2 is hydrogen content. Figure 6 shows the comparison of error of predicted value from ANN to calculated value from MLR and RSM at 750 °C. It can be obviously seen that the maximum errors from MLR and RSM are 46.7 and 45.6 MPa, respectively, while the maximum error from ANN is only 4.8 MPa, which suggests the errors from MLR and RSM are much higher than that from ANN. As a result, it can be evidently concluded that the prediction of present neural network model is in good agreement with the experimental data, and all the errors are within acceptable ranges which meet the integrity of the ANN learning and testing stages.

Combined influence of hydrogenation temperature and hydrogen content on tensile property of hydrogenated Ti600 alloy was plotted in the form of 3D, as shown in Fig. 7. It reveals that the tensile strength decreases with the increasing hydrogenation temperature and hydrogen content. From the comparison and analysis above all, it indicates that the ANN model can evaluate and predict the tensile properties of hydrogenated Ti600 alloy with sufficient accuracy and reliability, and the performing experiments according to the predicted value can provide a satisfactory and promising result.

The ultimate tensile strength (UTS) is given in the Eq 9 using ANN approach. The equation does not need adding experimental analysis and give a new formulation to determine the ultimate tensile strength. The UTS is calculated as follows:

$$\mathrm{UTS} = \frac{1}{1 + e^{-(1.09X_1 - 0.42X_2 - 0.54X_3 + 0.76X_4 - 0.72X_5 + 1.61X_6 - 1.71X_7 + 1.10X_8 + 0.37X_9 + 0.29X_{10} - 0.28)}} \quad \text{(Eq 9)}$$

where the transfer function used for this approach is given Eq 2. The values of X_i are given in Eq 10.

Table 2 Weights between input layer and hidden layer

	$X_i = w_{1i}K_1 + w_{2i}K_2 + w_{3i}$		
i	w_{1i}	w_{2i}	w_{3i}
1	−9.7395	−6.5323	11.9753
2	−11.82	0.0719	8.1646
3	−10.4089	−3.3748	9.3644
4	−9.9239	−7.8959	9.9232
5	10.0318	−5.457	−1.7852
6	4.4196	−11.2566	2.7629
7	1.4544	−12.0357	4.0038
8	−5.2332	−7.5236	4.3084
9	10.4723	−3.4098	−2.2347
10	3.4533	−10.0933	8.9903

$$X_i = w_{1i}K_1 + w_{2i}K_2 + w_{3i} \quad \text{(Eq 10)}$$

where the constants w_{ji} are given in Table 2, K_1 and K_2 are normalized values of hydrogenation temperature and hydrogen content, respectively.

5. Conclusions

A feed-forward BP neural network was established to exhibit the complex relationships between the tensile property and hydrogenation temperature and hydrogen content of hydrogenated Ti600 alloy. Satisfactory agreement between the experiment and the ANN results was obtained using this type of neural network, the maximum absolute error of predicted values is 4.8 MPa, and the relative error is within 5%. It shows that the neural network method has the advantage to treat the problem of multiple factors. A new equation of ultimate tensile strength as function of hydrogenation temperature and hydrogen content for hydrogenated Ti600 titanium alloy has been established. Compared with the conventional methods, it will save much cost and testing time. Hence, it can be concluded that ANN has great potential as novel prediction technique in the area of multi-variable and nonlinear system.

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References

1. O.N. Senkov and F.H. Froes, Thermohydrogen Processing of Titanium Alloys, *Int. J. Hydrogen Energy*, 1999, **24**, p 565–576 (in English)
2. K. Yang and D.V. Edmonds, Effect of Hydrogen as a Temporary Alloying Element on the Microstructure of a Ti3Al Intermetallic, *Scr. Metall. Mater.*, 1993, **28**, p 71–76 (in English)
3. Y. Furuya, A. Takasaki, K. Mizuno, and T. Yoshiie, Hydrogen Desorption from Pure Titanium with Different Concentration Levels of Hydrogen, *J. Alloys Compd.*, 2007, **446–447**, p 447–450 (in English)
4. D.B. Shan, Y.Y. Zong, Y. Lv, and B. Guo, The Effect of Hydrogen on the Strengthening and Softening of Ti–6Al–4V alloy, *Scr. Mater.*, 2008, **58**, p 449–452 (in English)
5. Y. Zhang, S.Q. Zhang, and C. Tao, Hydrogenation Behavior of Ti-25Al-10Nb-3V-1Mo Alloy and Effect of Hydrogen on its Microstructure and Hot Deformability, *Int. J. Hydrogen Energy*, 1997, **22**, p 125–129 (in English)
6. L.N. López de lacalle, J. Pérez, J.I. Llorente, and J.A. Sánchez, Advanced Cutting Conditions for the Milling of Aeronautical Alloys, *J. Mater. Process. Technol.*, 2000, **100**, p 1–11 (in English)
7. X.L. Wang, Y.Q. Zhao, and W.D. Zeng, *5th International Conference on Advanced Materials and Processing*, Sep 2008 (Harbin, China), Harbin Inst. Technol. p 863–868
8. Y. Niu, H.L. Hou, M.Q. Li, and Z.Q. Li, High Temperature Deformation Behavior of a Near Alpha Ti600 Titanium Alloy, *Mater. Sci. Eng. A*, 2008, **492**, p 24–28 (in English)
9. W. Sha and K.L. Edwards, The Use of Artificial Neural Networks in Materials Science Based Research, *Mater. Des.*, 2007, **28**, p 1747–1752 (in English)
10. H.K.D.H. Bhadeshia, R.C. Dimitriu, and S. Forsik, Performance of Neural Networks in Materials Science, *Mater. Sci. Technol.*, 2009, **25**, p 504–510 (in English)
11. Y. Sun, W.D. Zeng, Y.Q. Zhao, Y.L. Qi, X. Ma, and Y.F. Han, Development of Constitutive Relationship Model of Ti600 Alloy Using Artificial Neural Network, *Comput. Mater. Sci.*, 2010, **48**, p 686–691 (in English)
12. S. Mandal, P.V. Sivaprasad, S. Venugopal, K.P.N. Murthy, and B. Raj, Artificial Neural Network Modeling of Composition–Process–Property Correlations in Austenitic Stainless Steels, *Mater. Sci. Eng. A*, 2008, **485**, p 571–580 (in English)
13. W.D. Zeng, Y. Shu, and Y.G. Zhou, Artificial Neural Network Model for the Prediction of Mechanical Properties of Ti-10V-2Fe-3Al Titanium Alloy, *Rare Met. Mater. Eng.*, 2004, **33**, p 1041–1044 (in Chinese)
14. R. Rojas, *Neural Network, a Systematic Introduction*, Springer, Germany, 1996
15. Q. Li, J.Y. Yu, B.C. Mu, and X.D. Sun, BP Neural Network Prediction of the Mechanical Properties of Porous NiTi Shape Memory Alloy Prepared by Thermal Explosion Reaction, *Mater. Sci. Eng. A*, 2006, **419**, p 214–217 (in English)
16. J.T. Liu, H.B. Chang, T.Y. Hsu, and X.Y. Ruan, Prediction of the Flow Stress of High-Speed Steel During Hot Deformation Using a BP Artificial Neural Network, *J. Mater. Process. Technol.*, 2000, **103**, p 200–205 (in English)
17. M.H. Hassoun, *Fundamentals of Artificial Neural Networks*, The MIT Press, England, 1995
18. M.T. Hagan, H.B. Demuth, and M. Beale, *Neural Network Design*, Thomson Learning, Singapore, 2002
19. S. Malinov and W. Sha, Application of Artificial Neural Networks for Modelling Correlations in Titanium Alloys, *Mater. Sci. Eng. A*, 2004, **365**, p 202–211 (in English)
20. N.S. Reddy, Y.H. Lee, C.H. Park, and C.S. Lee, Prediction of Flow Stress in Ti-6Al-4V Alloy with an Equiaxed $\alpha+\beta$ Microstructure by Artificial Neural Networks, *Mater. Sci. Eng. A*, 2008, **492**, p 276–282 (in English)
21. O.N. Senkov and J.J. Jonas, Dynamic Strain Aging and Hydrogen-Induced Softening in Alpha Titanium, *Metall. Mater. Trans. A*, 1996, **27**, p 1877–1887 (in English)
22. Y. Niu and M.Q. Li, Effect of 0.16wt% Hydrogen Addition on High Temperature Deformation Behavior of the Ti600 Titanium Alloy, *Mater. Sci. Eng A.*, 2009, **513–514**, p 228–232 (in English)
23. A.A. Ilyin, M.Y. Kollerov, and I.S. Golovin, Hydrogen Influence on Plastic Deformation Mechanism of β-Titanium Alloys of Ti–Nb System, *J. Alloys Compd.*, 1997, **253–254**, p 144–147 (in English)
24. Y.Y. Zong, D.B. Shan, Y. Lu, and B. Guo, Effect of 0.3 wt%H Addition on the High Temperature Deformation Behaviors of Ti–6Al–4V Alloy, *Int. J. Hydrogen Energy*, 2007, **32**, p 3936–3940 (in English)
25. I. Weiss and S.L. Semiatin, Thermomechanical Processing of Alpha Titanium Alloys—an Overview, *Mater. Sci. Eng. A*, 1999, **263**, p 243–256 (in English)