Modeling of Correlation between Heat Treatment and Mechanical Properties of Ti–6Al–4V Alloy Using Feed Forward Back Propagation Neural Network

Junaidi SYARIF, Yan Pratama DETAK and Rizauddin RAMLI

Department of Mechanical and Materials Engineering, Universiti Kebangsaan Malaysia, Bangi, 43600 Selangor, Malaysia.
E-mail: syarif@vlsi.eng.ukm.my; detak@vlsi.eng.ukm.my; rizauddin@vlsi.eng.ukm.my

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A model for predicting mechanical properties of Ti–6Al–4V alloy has been developed and the Feed Forward Back Propagation (FFBP) as one type of algorithm of the Artificial Neural Network has been applied as the prediction system. Hardness, ultimate tensile strength (UTS), yield strength (YS) and elongation that are basic mechanical properties of Ti–6Al–4V alloy are predicted as a function of heat treatment process. Other tensile testing parameter, i.e. strain rate, is also considered in the model because increase of strain rate will increase UTS and YS, but will decrease elongation. Since the FFBP is a supervised system, it requires a lot of input and output data pairs for training process. The data are acquired from literatures and preprocessed before training. Performance of the model are evaluated by the Normalized Root Mean Square Error (NRMSE) and the Coefficient Correlation (R). The NRMSE and the R values of both training and validation parts show almost excellent values. Therefore, the model using the FFBP is appropriate to predict the mechanical properties of Ti–6Al–4V alloy.

KEY WORDS: prediction system; Ti–6Al–4V alloy; feed forward backpropagation neural network; mechanical properties; thermal and mechanical treatment.

1. Introduction

Ti–6Al–4V alloy is one type of titanium alloy that has excellent mechanical properties. In general, Ti–6Al–4V alloy consists of stable α and β phases at ambient temperature, because the alloy contains α former and β former such as Aluminium and Vanadium, respectively. Phases and microstructures of the alloy can be modified through heat treatment or mechanical treatment. For instance, the alloy will transform to full β phase when it is heated over temperature of 888°C which is known as β transus. From this region, the alloy will exhibit various transformations and will reveal various microstructures owing to rate of the cooling process. The alloy, which is annealed above β transus and is cooled by rapid cooling exhibits martensitic structure. On the other hand, slow-cooled alloy will have coarse (α+β) dual phase and the strength is lower than that of as-quenched alloy. It means that change of microstructure due to the heat treatment gives significant effect on the mechanical properties of the alloy. Since relationship among microstructure, mechanical properties and parameters of process of the alloy is complicated, experimental work is needed to investigate microstructures and mechanical properties of the alloy. It is known that materials and experimental work are high cost and also time will be consumed for experiment. Thus, another method such as simulation is thought to be an alternative method to clarify the relationship among microstructures, mechanical properties and parameters of process of the alloy. Therefore, an Artificial Neural Network (ANN) is suitable for predicting mechanical properties of the alloy, because the ANN can solve non-linear correlation such as-stated relationship. ANN is the statistical method which is referring the human brain principle. Although it is known that modeling method of the ANN is strongly dependent on algorithm of the model, the Feed Forward Back Propagation (FFBP) is the most popular and has been used by many researchers to solve the non-linear problems. It is because the FFPB has various architectures, learning algorithms and activation functions.

In this study, a model for predicting mechanical properties of the Ti–6Al–4V alloy has been developed using the ANN with the FFBP algorithm. Ultimate Tensile Strength (UTS), Yield Strength (YS), elongation (e) and the hardness are mechanical properties that will be predicted for the Ti–6Al–4V alloys, which are subjected to thermal and mechanical processes.

2. Materials and Methods

Modeling system for predicting the mechanical properties of the Ti–6Al–4V alloy has been developed by correlating four output items, i.e. UTS, YS, elongation and hardness with several input conditions as shown in Fig. 1. All of the samples were processed by two types of heat treatment,
e.g. annealing treatment (AT) and solution treatment with aging (ST+A). Samples for the AT were heated at temperature from 800 to 1100°C with interval of 50°C. Then, the samples were cooled by three different cooling rates, i.e. water quench (WQ), air cooling (AC) and furnace cooling (FC). The samples will be denoted by AT+WQ, AT+AC and AT+FC. On the other hand, ST+A samples were subjected to solution treatment at 925°C for 30 min and were cooled by various cooling rates, i.e. WQ and AC, and then aged at 525°C for 4 h. The samples will be denoted by ST-WQ+A and ST-AC+A. Beside the heat treatment processes, the other parameter of tensile test are determined, i.e. strain rates as an input condition. All of the samples are tensile tested using various strain rates from 10⁻²/s to 10⁻¹/s.

The development of the model is divided into three procedures, i.e. preprocessing, processing and post processing. The preprocessing is a process, which consists of collecting data from various sources and classifying them. In this study, the input and the output data pairs are collected from many published literatures, which show correlation between tensile properties and hardness after the heat treatment process. Since the data sources are published in graphical form, thus they must be put to discrete form based on the cartesian coordinate system. Number of all data are 8664 pairs and distribution for all outputs are shown in Fig. 2. Nevertheless, not all data can be obtained in form of variables as shown in Table 1. In order to increase validity of the system, selection and classification of input and output data pairs are the most important processes.

The processing is the process for scaling, training and validating the system using the classified data. Number and variance of the data are major factors for reaching an ideal system. If the variation of data is small, the ANN will show good performance for both of training and validation. The dispersed data pairs can broaden the standard deviation and will deteriorate the model of the network. Thus, it must be analyzed and be scaled by several methods. The scaling is not the essential step to the neural network, but it can influence the results of prediction. Generally, the scaling of the training data is done to reach a value of 1 for the standard deviation and value of 0 for the mean, which can be described using Eq. (1).

\[ y = (x - x_{mean}) \cdot \frac{y_{std}}{x_{std}} + y_{mean} \] ..........................(1)

where \( x_{mean} \) is mean value of input data, \( x_{std} \) is standard deviation of input data, \( y_{mean} \) is the mean value of output data and \( y_{std} \) is the standard deviation of output data.

Nevertheless, the scaling method can apply minimum and maximum values in input and output data pairs to obtain normalizing data from the range of \(-1 \) to 1. The normalization is described in Eq. (2).

\[ y_{norm} = 2 \cdot \frac{y - y_{min}}{y_{max} - y_{min}} \] ..........................(2)

where \( y_{norm} \) is the normalization result, \( y_{max} \) is the minimum value of the database dan \( y_{max} \) is the maximum value of the database. The data are divided into two parts; first part, which is containing 75% of total data for training and the other is used for validation process.

In this study, the FFBP is applied as the algorithm for predicting the mechanical properties of the alloy. It is known that the performance of the FFBP can be determined by adjusting the architecture, the activation function and the learning algorithm. General architecture of FFBP is shown in Fig. 3. It is a simple architecture, because the FFBP has three layers, which are called as input, hidden and output layers. In input layer, there are two neurons \( X_1 \) dan \( X_2 \) which indicate the input parameters of the network, i.e. temperature in heat treatment and strain rates, respectively. While the output node represents the output variables, i.e. UTS, yield strength, elongation and hardness. Number of hidden nodes in hidden layer can be adjusted according to the requirement. The model in this study use the number of nodes in hidden layer are adjusted from 5 to 50. Node \( b_1 \) and \( b_2 \) in hidden and output layer are biases, which have the value of 1. Weights between input layer and hidden layer is presented by \( w \), while weights between hidden layer and output layer is presented by \( W \). The multiplication of the

| Parameter         | Number of Data | Maximum | Minimum | Standard Deviation |
|-------------------|----------------|---------|---------|--------------------|
| Strain Rates (s⁻¹)| 2153           | 10²     | 10⁻³    | 0.86               |
| Temperature (°C)  | 2540           | 1099    | 798     | 85.76              |
| UTS (MPa)         | 651            | 1178    | 935     | 93.37              |
| Yield Strength (MPa)| 754          | 1117    | 842     | 100.6              |
| Elongation (%)    | 2146           | 17.72   | 1.42    | 4.48               |
| Hardness          | 1142           | 426     | 361     | 17.81              |

**Table 1.** Classification the quantity of data source for training and validating the network as a function of strain rates and annealing temperature.
input values and the weight will be summed and processed by activation function in each hidden and output nodes.

The activation function for the FFBP can be adjusted only in hidden and output layers. The modeling system used a tangent sigmoid pattern for the activation function in the hidden nodes and linear pattern for the output nodes. The tangent sigmoid function and the linear function are stated in Eq. (3) and linear function in Eq. (4), respectively.

The tangent sigmoid function and the linear function are used in the FFBP, e.g. the Conjugate Gradient, the Quasi Newton, the One Step Secant, the Polak Ribiere etc., the GDM and the LM represent a simple algorithm and a complicated algorithm, respectively. The difference of GDM and LM algorithms is in the method for updating the weights. The Gradient Descent with Momentum (GDM) and the Lavenberg Marquardt (LM) are used as the learning algorithm. Although there are a lot of learning algorithms in the FFBP, the LM shows the change in the NRMSE performance of the FFBP such as the LM and the GDM as function of nodes. Learning algorithms that applied nodes from 5 to 50 have been evaluated and compared for each number of nodes. It is found that the LM obviously demonstrates the smallest value of the NRMSE. The NRMSE slightly decreases and becomes constant at the 10 nodes and above for the LM. On the other hand, the NRMSE of the GDM fluctuates owing to the nodes. The smallest NRMSE of the GDM is laid on the 25 number of nodes.

\[ Z_n = \tanh(z_n) = \frac{2}{1 + \exp(-2x_n)} - 1 \quad (3) \]

where, \( Z_n \) is the output results of hidden node and \( z_n \) is the summation result of output hidden multiplied by weights between hidden layer and output layer, which are indicated in Eq. (6).

\[ y_n = b_2W_{bj} + \sum_{i=1}^{5} z_iW_{in} \quad (6) \]

Moreover, the Gradient Descent with Momentum (GDM) and the Lavenberg Marquardt (LM) are used as the learning algorithm. Although there are a lot of learning algorithms in the FFBP, e.g. the Conjugate Gradient, the Quasi Newton, the One Step Secant, the Polak Ribiere etc., the GDM and the LM represent a simple algorithm and a complicated algorithm, respectively. The difference of GDM and LM algorithms is in the method for updating the weights. The GDM uses gradient descent with momentum for updating the weights as described in Eq. (7).

\[ dX = mc \times dX_{prev} + br(1-mc) \frac{d_{perf}}{dX} \quad (7) \]

where \( dX \) is the change of weight and bias, \( mc \) is momentum constant, \( dX_{prev} \) is previous change to the weight and bias, \( lr \) is learning rate and \( d_{perf}/dX \) is the derivatives of performance. Whereas LM uses Lavenberg Marquardt optimisation for updating the weight and bias through calculating the Jacobian of the performance. The algorithm of LM are shown in Eqs. (8) to (10).

\[ jy = jX \times jX \quad (8) \]

\[ je = jX \times E \quad (9) \]

\[ dX = -(jy + I \times mu) / je \quad (10) \]

where \( jX \) is the Jacobian, \( E \) is all errors, \( I \) is identity matrix and \( mu \) is initial \( mu \).

Since the input and output data pairs are very, all data can not be processed in one network, but they are divided into 6 networks according to their values. Validity of the model can be evaluated from the performance of both training and validation process. In order to asses the performance of the network, the Normalized Root Mean Square Error (NRMSE) and the Coefficient Correlation (R) are used in this study. The NRMSE is the difference of output target and output model, which is normalized by the output target, as shown in Eq. (11),

\[ \text{NRMSE} = \left( \frac{1}{t} \sum_{j=1}^{t} (Y'_j - Y_j)^2 \right)^{1/2} \quad (11) \]

where, \( Y'_j \) is the predicted output, \( Y_j \) is the actual target output, \( t \) is the number of training data pairs, and \( j = 1, 2, 3, \ldots, t \). While \( R \) is the strength of linear relationship between output target and output prediction, which is defined by their covariance normalized by their standard deviation as shown in Eq. (12),

\[ R(Y' - Y) = \frac{\text{cov}(Y' - Y)}{\sigma_{Y'} \sigma_Y} \quad (12) \]

where \( R(Y' - Y) \) is the coefficient correlation between predicted output and target, \( \text{cov}(Y' - Y) \) is the covariance between predicted output and target and \( \sigma_{Y'} \), \( \sigma_Y \) are the standard deviation of predicted output and target. The best performance of the network is indicated by minimum value of the NRMSE and value close to 1 of the \( R \).

Lastly, the post processing is the process for displaying results of the prediction. Since both of training and validation data are taken from graphical form, thus the results of prediction can be displayed by graphs. The experimental and prediction data are presented and are compared by lines and several shapes of plots, respectively. The graphs only show the validation part, which indicates the network testing using new input and output data pairs.

3. Results and Discussion

3.1. Performance of the Network

Simulation for verifying the performance of the system has been carried out. Figure 4 shows the change in the NRMSE performance of the FFBP such as the LM and the GDM as function of nodes. Learning algorithms that applied nodes from 5 to 50 have been evaluated and compared for each number of nodes. It is found that the LM obviously demonstrates the smallest value of the NRMSE. The NRMSE slightly decreases and becomes constant at the 10 nodes and above for the LM. On the other hand, the NRMSE of the GDM fluctuates owing to the nodes. The smallest NRMSE of the GDM is laid on the 25 number of nodes.
nodes, and it shows the best performance of GDM. However, the value of the GDM is obviously higher than that of the LM. It means that the LM will acquire better performance than the GDM for the learning algorithm. Figure 5 shows the R values of the networks, which are modeled using the LM and the GDM learning algorithms. Both of algorithms exhibit that values of the R are close to 1. However, the R values calculated by the GDM abruptly decrease when the nodes are 40 and above. Therefore, the results of the NRMSE and the R indicate that the LM has better performance for prediction than the GDM. The system for predicting mechanical properties of the Ti–6Al–4V alloy will utilize the LM as the learning algorithm. Since the values of the NRMSE and the R for the LM are almost constant for all nodes, thus the system will apply 25 nodes only.

3.2. Ultimate Tensile Strength and Yield Strength

Figure 6 shows the UTSes of the Ti–6Al–4V alloys as function of strain rates from $10^{-7}/s$ to $10^{-3}/s$. All of the samples are subjected to various ST+A treatments. The samples are water-quenched and air-cooled after solution treatment at 925°C and then aged at 525°C. The processes will be designated as ST-WQ+A or ST-AC+A process. The experimental results of ST-WQ+A process and ST-AC+A process are shown by the solid line and dash line, respectively. The graphs indicate that change of the strain rate will vary the UTS of the alloy. The UTS increases with increasing strain rate. It can be shown that the UTS of the water-quenched samples is higher than that of the air-cooled ones. The FFBP has been used for predicting relation between the UTS and the strain rate of the Ti–6Al–4V alloys, which have been subjected to various heat treatments. Circle and square plots in Fig. 6 show results of prediction for ST-WQ+A and ST-AC+A samples. Accurate results can be obtained because the circle and square plots are lying on the lines, which are the experimental results. Thus, it is thought that the FFBP can predict relation between the UTS and the strain rate.

Yield strength for Ti–6Al–4V alloys as function of strain rates are shown in Fig. 7. From the graphs, the yield strength will increase as the strain rates increase. The heat treatments, which are applied for samples in Fig. 6, are also used for the samples in Fig. 7. The heat treatments are called as the ST-WQ+A and the ST-AC+A. The yield strength of the ST-WQ+A is higher than that of the ST-AC+A samples. A prediction system has been developed using the FFBP to predict the relation between yield strength and the strain rate for Ti–6Al–4V alloys, which are heat treated. Figure 7 has shown the predicted results in circle and square plots within the graph. All of the predicted values are lying on the experimental results, i.e. the lines. Thus, it is proved that the prediction system by the FFBP is also suitable for predicting yield strength of the Ti–6Al–4V alloy. The results for UTS and yield strengths are reported by Venkatesh et al. 4)

3.3. Elongation

Elongation is one of the tensile properties that shows ductility of the materials and usually shows trade-off relation with the strength. The Ti–6Al–4V alloys have specific elongation depending on fabrication of the alloy. The ST+A and the AT are well-known as the heat treatments,
which can influence ductility of the alloy. Figure 8 shows relation between annealing temperature of the AT process and elongation. It was reported that the elongation of the alloy, that was heat-treated at β transus and above are lower than that of one, which was heat-treated below β transus. It is also shown that cooling rate gives significant influence to the ductility. The elongation decreases with increasing cooling rate. The experimental results of Fig. 8 are published by Jovanovic et al. A model for predicting the elongation of Ti–6Al–4V alloy has been developed and the result is also shown in Fig. 8. The results of the effect of WQ, AC and FC are plotted in circle, square and triangle shapes, respectively. All of the predictions plots are lying on the lines.

Since the elongation also changes owing to the strain rate, a model for predicting relation between the elongations and strain rates is also developed. The alloy was subjected to aging after ST process with cooling at various rates. Figure 9 shows the relation between the elongation and strain rate of the Ti–6Al–4V alloy, which was subjected to the STA process. The experimental data were published by Venkatesh.

The elongations of all samples exhibit almost the same behavior; the elongations decrease with increasing strain rate. Prediction of the elongations for the ST-AC + A and the ST-WQ + A samples are also done and the results are shown in square and circle plots. It is found that elongation predicted results are almost on the same position with the experimental results, i.e. solid line and dashed line.

From the above results, the relation among the heat treatments, tensile test parameter and tensile properties, e.g. the UTS, the yield strength and the elongation can be clarified and the tensile properties of the alloy can be predicted using the FFBP.

3.4. Hardness

Although it is known that hardness has strong relationship with the UTS, it is also important to develop system that can identify correlation between thermal and mechanical treatments and hardness of the Ti–6Al–4V alloy. Figure 10 shows relation between hardness and annealing temperature of the Ti–6Al–4V alloy. The hardness increased when annealing temperature increases or cooling rate after the AT process increases. Results of prediction of hardness using FFBP are shown, within Fig. 10. The results are plotted by open circle, open square and open triangle plots for the AT-WQed, AT-ACed and AT-FCed samples, respectively. The position of the plots are precisely lying on the lines. From these results, correlation between heat treatment, the mechanical properties of the alloy and strain rate of tensile test can be clarified and the system for predicting the mechanical properties as output can be developed using the FFBP as the algorithm with heat treatment process and strain rate as the input.

4. Conclusions

The heat treatment process can be used to control the mechanical properties of Ti–6Al–4V properly. From the tensile test results, it has been shown that water quench gives the significant effect for influencing the UTS and YS, but decreasing the elongation. Likewise the influence of strain rates will increase the UTS and YS and decrease the elongation. The increasing temperature of annealing also can be used to increase the hardness of the alloy.

The modeling system for predicting mechanical properties of Ti–6Al–4V alloy has been developed using FFBP algorithm. Two different learning algorithms, that are GDM and LM, are trained and compared to generate the proper prediction model. The NRMSE, which explain that LM has smaller value than GDM, gives the evidence that LM is more suitable to be set as the learning algorithm. Moreover, the \( R \) value of LM is constant at the ideal condition. From the number of hidden nodes, the ideal model can be achieved when the number of nodes in hidden layer are 25. Therefore the prediction model is built using LM learning algorithm with 25 number of nodes inside hidden layer.

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