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Modeling the Correlation of Composition-Processing-Property for TC11 Titanium Alloy Based on Principal Component Analysis and Artificial Neural Network

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In the present investigation, the correlation of composition-processing-property for TC11 titanium alloy was established using principal component analysis (PCA) and artificial neural network (ANN) based on the experimental datasets obtained from the forging experiments. During the PCA step, the feature vector is extracted by calculating the eigenvalue of correlation coefficient matrix for training dataset, and the dimension of input variables is reduced from 11 to 6 features. Thus, PCA offers an efficient method to characterize the data with a high degree of dimensionality reduction. During the ANN step, the principal components were chosen as the input parameters and the mechanical properties as the output parameters, including the ultimate tensile strength (σ_b), yield strength ($\sigma_{0.2}$), elongation (δ), and reduction of area (φ). The training of ANN model was conducted using back-propagation learning algorithm. The results clearly present ideal agreement between the predicted value of PCA-ANN model and experimental value, indicating that the established model is a powerful tool to construct the correlation of composition-processing-property for TC11 titanium alloy. More importantly, the integrated method of PCA and ANN is also able to be utilized as the mechanical property prediction for the other alloys.

Keywords mechanical property, neural network, principle component analysis, processing parameters, TC11 titanium alloy

1. Introduction

As a typical $\alpha + \beta$ heat resistance titanium alloy, TC11 alloy possesses the excellent thermal stability, high temperature strength, and creep property besides the common advantages, such as low density, high strength-to-weight ratio, and corrosion resistance. It is mainly applied to manufacture the critical components for aero engines, including compressor disks and blades. In the past few years, a variety of investigations have been conducted with respect to TC11 titanium alloy by the materials scientists throughout the world. Zong et al. (Ref 1) evaluated the constitutive behavior and the microstructural evolution of TC11 alloy under hot processing conditions for the sake of optimizing its hot workability and controlling the microstructure. Chen et al. (Ref 2) studied the hot deformation behaviors of TC11 alloy with β-annealed lamellar structure and forged equiaxed structure in the β-phase region in the temperature range of 1030-1090 °C and strain rate range of 0.001-0.1 s^{-1} by means of isothermal compression tests. Song et al. (Ref 3) primarily investigated the effect of deformation conditions on deformation mechanisms of TC11 alloy during subtransus processing for better understanding of the relationship between the processing condition and microstructure evolution. Sun et al. (Ref 4) developed the optimization model of chemical composition for TC11 titanium alloy using combined artificial neural network (ANN) and genetic algorithm. Based on the systemic investigations mentioned above, it can in fact be revealed that the mechanical properties of TC11 titanium alloy are quite sensitive to its chemical composition and hot processing parameters. As a result, it is significant to understand the correlation of composition-processing-property so that the alloy composition and processing parameters could be optimized to achieve desirable mechanical properties. However, the relationship of composition, processing, and property presents extremely complex and highly nonlinear. The quantitative analysis of the relationship between them cannot be carried out exclusively by the conventional experimental approach. Although the statistical techniques like multilinear regression method are beneficial to resolve the multivariable and nonlinear problems, they are quite time- and labor-consuming types of work to obtain the constants and their predicted accuracies are also limited.

Recently, ANN is able to simulate certain intelligent behavior of human brain, which possesses the abilities of self-learning, self-organizing, self-adaptive, high fault-tolerance and accurate description of nonlinear problems. ANN has strong superiority in terms of resolving the complicated problems which are characterized by multivariable, highly nonlinear system and implicit function relation. Even if there are no sufficient experimental datasets, the complex correlation of composition-processing-property of materials can be still

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elaborated. On the basis of its obvious advantages, ANN technique has been successfully and extensively applied in the various fields of metals and alloys, including prediction of mechanical properties (Ref 5–8), optimization of processing parameters (Ref 4, 9–11), and the establishment of constitutive relationship (Ref 12–14). Nevertheless, with the increase of the number of input variables and sample data, the structure of neural network might be more complicated and the problem of over-fitting would happen, which restrict the precision of prediction and the learning rate of neural network. Consequently, the principal component analysis (PCA) method was adopted to reduce training data and simplify the network structure under the premise of insuring the predicted accuracy of the established model. For instance, Agarwal et al. (Ref 15) successfully identified various phases and phase-groups using the combined method of PCA, genetic algorithm and ANN based on a large number of AB_2 compounds. Therefore, the main objective of this study is to model the correlation of composition-processing-property of TC11 titanium alloy based on the combination techniques of PCA and ANN. The comparison of the potential performance of PCA-ANN and ANN approaches was conducted to evaluate their respective availability. The developed network model will be beneficial to the other alloys also in terms of composition design and processing optimization.

2. Theory of Principal Component Analysis and Artificial Neural Network

2.1 Principle Component Analysis

As a mathematical technique, PCA utilizes an orthogonal linear transformation to convert a set of observations of possibly correlated variables into a set of values of uncorrelated variables called principal components. In other words, PCA is a kind of statistical approach which is designed to reduce the number of variables to a small number of indices while attempting to preserve the relationships present in the original data more rapidly and effectively. Basically, the number of principal components is less than or equal to the number of primary variables. Therefore, the PCA method is considered to be the simplest of the true eigenvector-based multivariable analyses, which is able to reveal the internal structure of the data, which well interprets the variance in the datasets (Ref 16–18). The implementation of PCA method is shown in Fig. 1.

The basic principle of PCA method can be explained as follows. Suppose that there are evaluating indicators numbering m, evaluating objects numbering n, the value of the jth object on the ith evaluating indicator is represented as x_{ij}, and an original indicator value matrix $x_{(ij)m\times n}$ is formed. This matrix should be normalized as

$$\tilde{x} = \frac{x_{ij} - \bar{x}_j}{S_j} \quad (i = 1, 2, \ldots, n;\ j = 1, 2, \ldots, p) \qquad \text{(Eq 1)}$$

where $\bar{x}_j$ is the mean value of the sample, and S_j is the sample standard deviation of x_j. Then, the correlation coefficient matrix $R = (r_{ij})_{m\times n}$ is achieved, where x_{ij} is the data of jth evaluating object on the indicator and $r_{ij} \in [0, 1]$. In order to construct m-dimensional new evaluating variables as Eq 1, the eigenvalue of correlation coefficient matrix $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0$ and the corresponding eigenvector $a_1, a_2, \ldots, a_m$ are calculated.

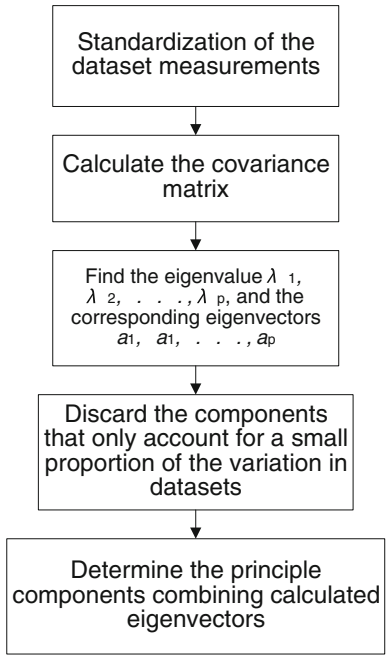

Fig. 1 The flow chart of PCA

$$\begin{cases} y_1 = a_{11}\tilde{x}_1 + a_{21}\tilde{x}_2 + \cdots + a_{m1}\tilde{x}_m \\ y_2 = a_{12}\tilde{x}_1 + a_{22}\tilde{x}_2 + \cdots + a_{m2}\tilde{x}_m \\ \cdots \\ y_m = a_{1m}\tilde{x}_1 + a_{2m}\tilde{x}_2 + \cdots + a_{mm}\tilde{x}_m \end{cases} \qquad \text{(Eq 2)}$$

where y_m is the m principal component. It is the last step for the calculation of the informative contribution rate and accumulated contribution rate represented by Eq 3 and 4, respectively.

$$b_j = \frac{\lambda_j}{\sum_{k=1}^{m}\lambda_k} \qquad \text{(Eq 3)}$$

$$\alpha_p = \frac{\sum_{k=1}^{p}\lambda_k}{\sum_{k=1}^{m}\lambda_k} \qquad \text{(Eq 4)}$$

where b_j is the informative contribution rate of principal y_j, and α_p is the accumulated contribution rate of principal $y_1, y_2, \ldots, y_p$. When the value of α_p is more than 0.8, it can be thought that the whole procedure of PCA is terminated.

2.2 Artificial Neural Network

ANN is normally a robust and parallel computing system, which is composed of many simple and interconnected processing units (neurons) that usually do little more than take a weighted sum of all their inputs. It is suitable for ANN model to process information by its internal dynamic response to external inputs (Ref 19). The applications scope of ANN derives from their excellent capability to estimate complicated relation functions that make them applicable and compatible for modeling nonlinear relationships. The detailed introduction to the basic algorithm concerning ANN could be found and deeply understood in the literature (Ref 19, 20). For the purpose of better application of ANN model, it is quite necessary and

Table 1 Selected data information of chemical composition, processing, and property of TC11 alloy

Chemical composition									Processing parameter		Mechanical properties			
Al	Mo	Zr	Si	Fe	C	H	O	N	Forging temperature, °C	Cooling style(a)	Ultimate tensile strength, MPa	Yield strength, MPa	Elongation, %	Reduction of area, %
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	970	2	1070	1030	16	48.6
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	970	2	1060	1000	16.4	42.1
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	970	1	1120	1040	13.2	40.2
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	970	1	1080	1050	14	36.5
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	990	2	1100	1040	14	45
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	990	2	1080	1040	14.5	48
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	990	1	1080	1040	10.8	43.5
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	990	1	1080	1030	10.8	45
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	1010	2	1130	1040	16.4	30.4
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	1010	2	1090	1040	8.8	26.5
6.41	3.46	1.58	0.31	0.08	0.05	0.008	0.009	0.018	1010	1	1100	1050	8.4	19.5
6.41	3.46	1.58	0.31	0.08	0.015	0.008	0.009	0.018	1010	1	1080	1030	8.4	25
6.52	3.5	1.58	0.26	0.073	0.013	0.0006	0.1	0.01	1000	1	1030	970	16	39.3
6.52	3.5	1.58	0.26	0.073	0.013	0.0006	0.1	0.01	1010	1	1080	1000	15	38
6.52	3.5	1.58	0.26	0.073	0.013	0.0006	0.1	0.01	1020	1	1050	995	14.8	28.8
6.52	3.5	1.58	0.26	0.073	0.013	0.0006	0.1	0.01	1030	1	1070	980	13	25
6.25	3.51	1.58	0.21	0.052	0.045	0.0005	0.065	0.017	990	2	1120	1040	13	47.8
6.25	3.51	1.58	0.21	0.052	0.045	0.0005	0.065	0.017	1010	2	1090	980	12.5	26.3
6.34	3.52	1.92	0.28	0.072	0.02	0.0028	0.097	0.01	950	2	1090	955	13.6	43
6.46	3.5	1.92	0.28	0.12	0.02	0.0022	0.102	0.008	970	2	1080	890	16	36.6

(a) 1—air cooling, 2—water cooling

meaningful to describe feed-forward network trained by back-propagation (BP) learning algorithm. In general, BP algorithm is a sort of generalized form of the least mean squares algorithm. By means of utilizing the algorithm-generalized gradient descent search technique, the BP algorithm adjusts the weights of the network and the threshold of each neuron recurrently on the basis of the minimization of the mean square error (MSE) criterion is minimized. Theoretically, BP neural network which is composed of an input layer, a hidden layer, and an output layer may approach any continuous functional relationship in any closing region (Ref 21). Thus, a three-layer neural network model is employed in the present investigation. Furthermore, the appropriate number of hidden-layer neurons is a critical parameter affecting the performance of the neural network model. Thus, the repetitive trial approach will be adopted to obtain the optimal network structure and prediction performance.

Table 2 Statistical analysis of the input datasets for ANN model

	Minimum value	Maximum value	Mean value	Standard deviation
Al, wt.%	5.82	6.83	6.36	0.260
Mo, wt.%	2.97	3.63	3.38	0.149
Zr, wt.%	1.48	1.96	1.71	0.140
Si, wt.%	0.21	0.40	0.29	0.036
Fe, wt.%	0.03	0.12	0.07	0.019
C, wt.%	0.002	0.06	0.025	0.015
H, wt.%	0.0005	0.01	0.004	0.003
O, wt.%	0.007	0.122	0.078	0.038
N, wt.%	0.004	0.15	0.024	0.038
Forging temperature, °C	950	1030	984	0.205
Cooling style(a)	1	2	1.80	0.402

(a) 1—air cooling, 2—water cooling

3. Modeling the Correlation of Composition-Processing-Property for TC11 Titanium Alloy

3.1 Data Acquisition and Preprocessing

Basically, the accuracy and applicability of a neural network model is considerably affected by the quality and size of the training dataset. In the present research, an amount of data on mechanical properties of TC11 titanium alloy under various conditions of forging processing are listed in Table 1. It is necessary to note that the forging testing was carried out on the 25T-M counter-blow hammer, and the tensile testing at room temperature was conducted on the Zwick/Z150 universal testing machine with initial tensile rate of 0.6 mm/min. However, the collected datasets are rather confusing and in disorder for utilization of engineering practice. It is inevitable to perform the procedure of analysis and preprocessing on the training data. Table 2 lists the detailed information of input datasets for the ANN model in a primary statistical term. It is observed from Table 1 that the minimum and maximum values of standard deviation are, respectively, 0.003 and 0.402, which indicate that the collected datasets are available for the ANN model.

Table 3 The eigenvalues of covariance matrix and their accumulated contribution rate

i	1	2	3	4	5	6	7	8	9	10	11
λ_i	2.55	2.01	1.83	1.06	1.02	0.78	0.69	0.44	0.31	0.19	0.12
Q_m, %	23.18	41.37	58.00	67.64	77.00	84.10	90.37	94.41	97.19	98.93	100

In order to reduce the dimensions of the input data and simplify the network structure, PCA was employed for the preprocessing of the training data after confirming the data acquisition. The eigenvalue (λ_i) and accumulated contribution rate (α_p) of covariance matrix are shown in Table 3. From this table, it can be observed that the λ_6 and α_6 of the sixth principal component are 0.78 and 84.10%, respectively, which suggests that the characterization of data sample has been mainly extracted. The value of α_6 is very close to 1, implying such principal components are able to present the characterization information completely. More importantly, the dimension of the training dataset is greatly reduced from 11 to 6, which significantly facilitates the simplification of the network size.

3.2 Training and Verifying the Neural Network

In order to balance the weight of each input and output parameter as well as alleviate the training difficulty of the network during training process, it is necessary to normalize the training data. In general, it is strongly recommended that the data be unified between slightly offset values such as from 0.1 to 0.9 rather than between 0 and 1, so as to avoid saturation of the sigmoid function bringing about slow or no learning. The method of normalization is extensively used as

$$Z_i = 0.1 + 0.8 \times \left(\frac{Z - Z_{\min}}{Z_{\max} - Z_{\min}} \right) \quad \text{(Eq 5)}$$

where Z_i is the normalized data of the corresponding to Z, and $Z_{\min}$ and $Z_{\max}$ are the minimum and maximum values of Z, respectively. Subsequently, 85 of the datasets were randomly selected as training set, and the remaining five of datasets were used for verifying the trained network model. Figure 2 shows the correlation of composition-processing-property for TC11 titanium alloy in the form of schematic implementation. As shown in this figure, the fully connected multilayer feed-forward neural network is composed of three layers, including one input layer, one hidden layer and one output layer. The numbers of neurons present in the input and output layers are associated with the number of different variables. In the present study, the input variables of the network model are the first and the second principal components based on the chemical compositions (Al, Mo, Zr, Si, Fe, C, H, O, and N) and processing parameters (forging temperature and cooling style). The output variables of ANN are the mechanical properties, including ultimate tensile strength (σ_b), yield strength ($\sigma_{0.2}$), elongation (δ), and reduction of area (φ). The number of the hidden-layer neurons of ANN model was acquired by trial-and-error approach from 5 to 20. Figure 3 shows the influence of the number of neurons in hidden layer on the performance of the network. It is found that when the neurons in the hidden layer reached 15, the ANN model represented optimum performance which was quantitatively evaluated by the term of MSE. The tansig and logsig were chosen as the transfer functions used for

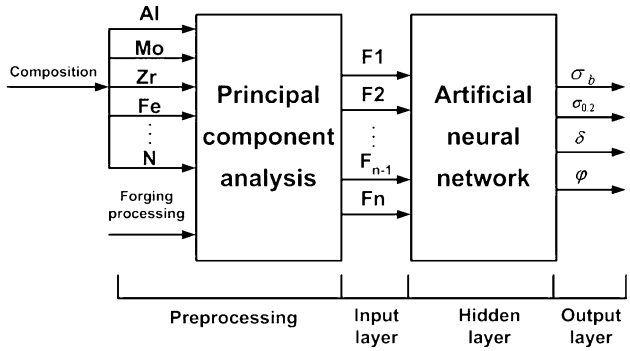

Fig. 2 Schematic implementation of the development of the correlation of composition-processing-property for TC11 titanium alloy

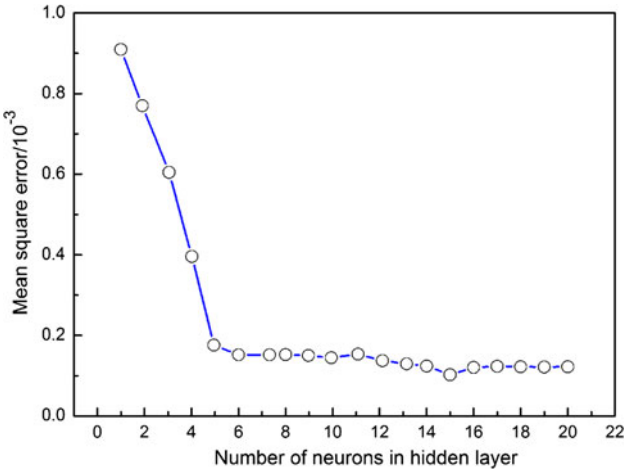

Fig. 3 Influence of the number of neurons in hidden layer on the performance of the network

input-hidden layer and hidden-output layer, respectively. Also, the trainlm algorithm was found to train the ANN model in a robust and fast way. During the training step, the whole calculation of the neural network was performed with a training set using MATLAB 7.4® software. The ANN model correlated the input and output variables by searching for the most desired set of weights to minimize the objective function.

4. Results and Discussion

In the present research, composition-processing-property of TC11 titanium alloy were first correlated using ANN model, and then the PCA-ANN correlation developed above was used for the properties estimations from the alloy compositions and hot processing parameters. Furthermore, attempts were also made to compare prediction accuracies of ANN and PCA-ANN correlation model, and thus to provide a set of reliable tool for

the quality control of TC11 titanium alloy. During the training procedure, the ANN achieved a stable state after 658 iterative cycles. The comparison result of ANN and PCA-ANN model for the composition-processing-property of TC11 titanium alloy is listed in Table 4. It is observed from this table that the dimension of the input layer has been greatly simplified after the PCA process, which directly affects the size of the network model. Thus, it can be considered that the development of the correlation model of composition-processing-property for TC11 alloy has been optimized based on the PCA-ANN approach. The evaluation of the performance of the training network is quantified by correlation coefficient (R), which is defined as

Table 4 Compared result of ANN and PCA-ANN model for the composition-processing-property of TC11 titanium alloy

	Number of input-layer neurons	Number of hidden-layer neurons	Training epochs/goal error	Correlation coefficient
ANN model	11	15	5000/0.001	0.825
PCA-ANN model	6	15	658/0.001	0.936

$$R = \frac{\sum_{i=1}^{N}(E_i - \bar{E})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{N}(E_i - \bar{E})^2 \sum_{i=1}^{N}(P_i - \bar{P})^2}} \quad \text{(Eq 6)}$$

where N is the total number of data employed in the investigation. E is the experimental value, and P is the predicted value obtained from the neural network model. $\bar{E}$ and $\bar{P}$ are the mean values of E and P, respectively. Figure 4 depicts a comparison of the experimental versus predicted data point with PCA-ANN using training datasets. It is indicted that 90% of the data points are quite close to the line inclined at 45° to the horizon, and the R value is found to be more than 0.918, suggesting that the accuracy of the predicted mechanical properties based on the PCA-ANN model is preferable, and a good agreement between the predicted and experimental data has been achieved by the established model. Therefore, the trained neural network is able to successfully predict the mechanical properties of TC11 alloy. In order to further study the prediction performance of the present model, the analyses of the mean of absolute relative error (MARE) and mean of absolute error (MAE) were carried out, which are described as follows:

$$\text{MARE}\ (\%) = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{E_i - P_i}{E_i}\right| \times 100 \quad \text{(Eq 7)}$$

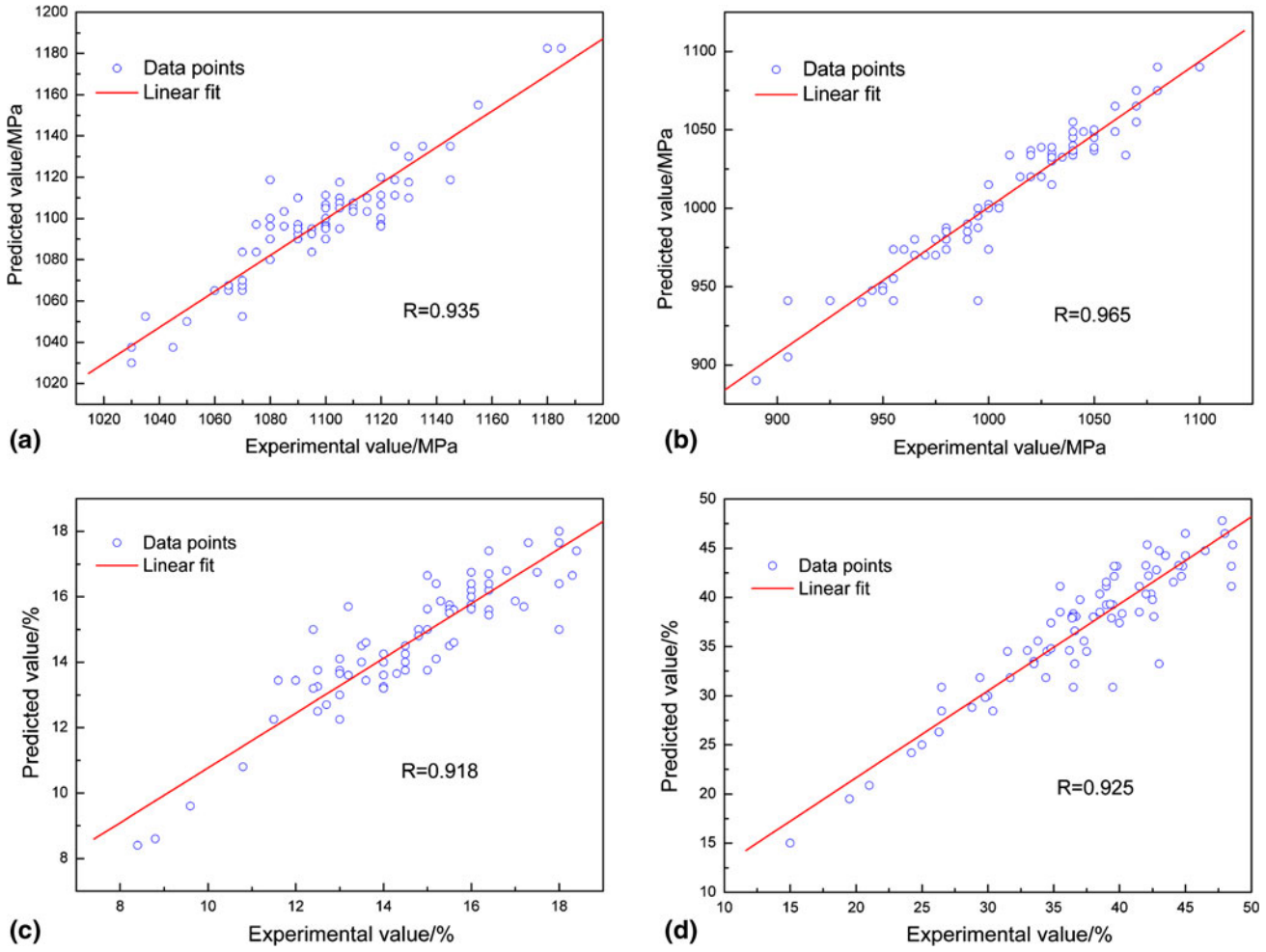

Fig. 4 Comparison of predicted mechanical properties for TC11 titanium alloy by the ANN model with experimental value: (a) ultimate tensile strength, (b) yield strength, (c) elongation, and (d) reduction of area

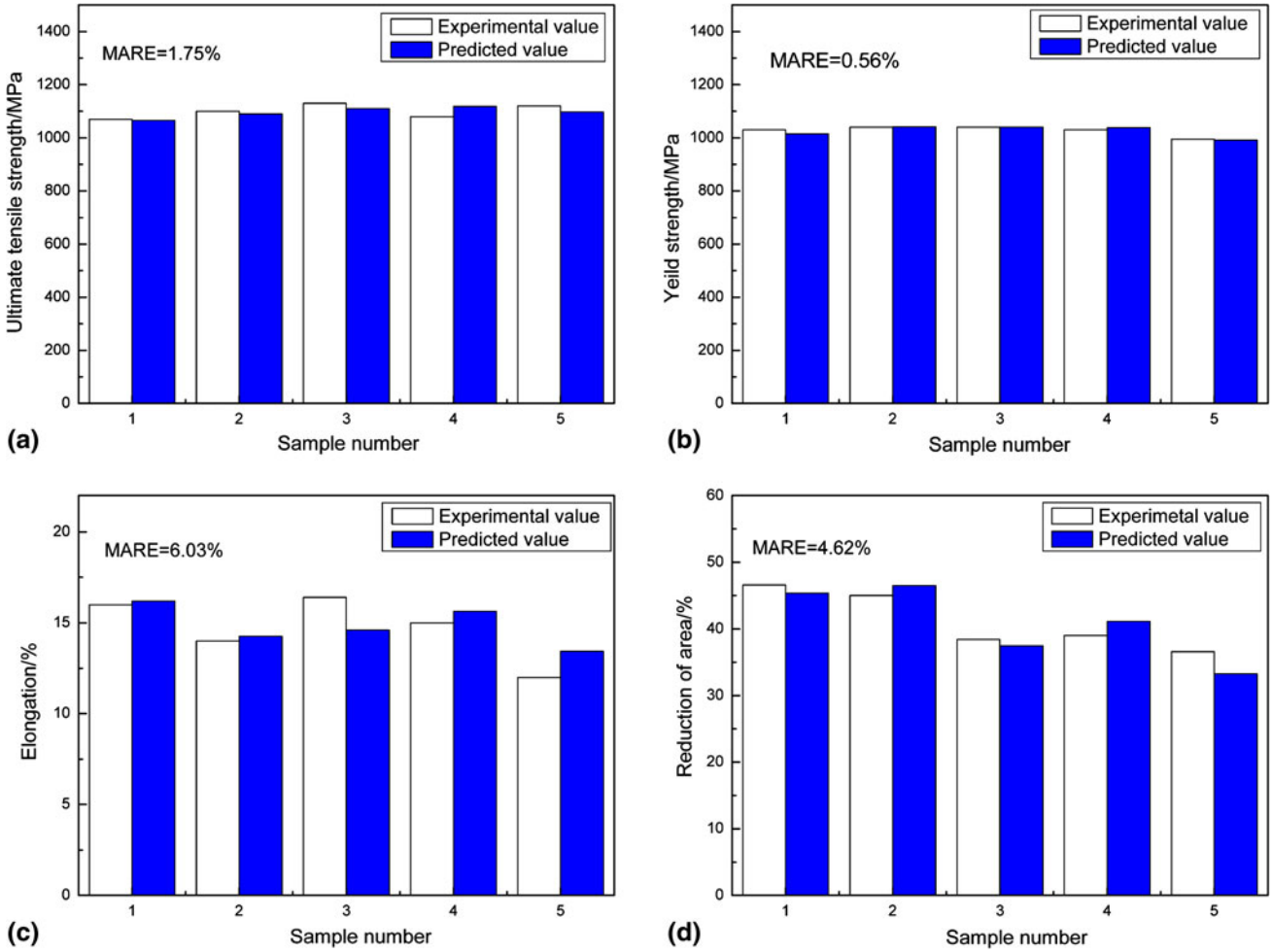

Fig. 5 Analysis of mean average relative error (MARE) between predicted value by ANN and experimental value: (a) ultimate tensile strength, (b) yield strength, (c) elongation, and (d) reduction of area

$$\text{MAE (MPa)} = \frac{1}{N}\sum_{i=1}^{N}|P_i - E_i| \qquad \text{(Eq 8)}$$

Figure 5 presents the mechanical properties of TC11 alloy predicted from the ANN model compared with the experimental values. It is clearly observed from this figure that the relative errors between the predicted and the experimental values are all less than 6.5%, which implies that the satisfactory prediction results of ANN model can be achieved. In addition, the MARE and MAE are 3.24 and 6.94, respectively. Hence, it is concluded that the established correlation model based on the PCA and ANN can be used to predict the mechanical properties and optimize hot processing parameters of TC11 titanium alloy.

5. Conclusions

In the present investigation, on the basis of the large number of the experimental datasets obtained from the forging experiments under various conditions of chemical composition and forging processing, the correlation of composition-processing-property of TC11 titanium alloy was successfully developed, using the combined techniques of PCA and ANN. It was found that the PCA method was performed for robust feature extraction from the input variables. After the PCA process, the dimension of the feature vector significantly reduced from 11 to 6, which contains most of the useful information from the original vector. Meanwhile, a powerful correlation model between the principal components and mechanical properties of TC11 titanium alloy was constructed with the help of application of ANN approach trained with the BP learning algorithm. The MARE and MAE are only 3.24 and 6.94, respectively, which firmly suggests that the predicted values are in quite good agreement with the experimental values. Therefore, the developed correlation model on composition-processing-property is a more promising solution for the optimization of processing parameter and control of mechanical property with high reliability. In the future researches, the PCA-ANN intelligent approach can be applied to the other alloys. Also, the additional information such as a variety and a number of affecting factors can be taken into consideration.

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