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Artificial neural network modeling on the relative importance of alloying elements and heat treatment temperature to the stability of α and β phase in titanium alloys

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ABSTRACT

An artificial neural network model was developed to correlate the relationship between the alloying elements (Al, V, Fe, O, and N) and heat treatment temperature (inputs) with the volume fractions of α and β phases (outputs) in some α, near-α, and α + β titanium alloys. The individual and combined influences of the composition and temperature on α and β phases were simulated through performing sensitivity analysis. A new method has been proposed to estimate the relative importance of the inputs on the outputs for single phase α-Ti, near-α Ti, and α + β Ti alloys. The average error of the model predictions for 35 unseen test data sets is 1.546%. The estimated behavior of volume fractions of α and β phases as a function of composition and temperature are in good agreement with the experimental knowledge. Justification of the results from the metallurgical interpretation has been included.

1. Introduction

The titanium alloys are garnering significant engineering importance due to their high strength-to-weight ratio and excellent corrosion resistance [1,2]. Generally, Ti alloys have different volume fractions of α and β phases depending on the composition, heat treatment, and interstitial content. The ratio of α and β phases and their distribution determines the mechanical and thermal properties. The α phase has HCP structure with limited slip system, which results in low ductility, relatively high strength and excellent creep resistance. In contrast, β phase has BCC structure with moderate ductility and strength. The titanium alloys can acquire a large variety of microstructures with different geometrical arrangements of α and β phases. They can be classified into three different categories: lamellar, equiaxed, or a mixture, i.e. bimodal. The relationship between α and β phase volume fractions with the composition and heat treatment temperature is very sensitive and complex in nature.

Artificial neural networks (ANN) techniques applied in predicting the various phenomenon of alloys due to their ability to learn input–output relationships for the complex problems [3–6]. The most important feature is that ANN do not require specific equation forms. They only require sufficient meaningful input–output data. The capability of ANN models as universal function approximators has been used to solve the problems in which the relationship is unclear between the dependent and independent variables. ANNs have been successfully applied to numerous applications in material science [7–10]. ANN models have been used in different phenomenon such as prediction of flow stress of Ti600 alloy [11], creep behavior of IMI 834 alloy [12], correlating microstructure with properties [7,13] and β transus temperature [14,15]. However, the available literature is limited to predict various phenomena of specific titanium alloy and the role of alloying elements has not been reported quantitatively.

The primary objectives of the present study are: (i) to predict the volume fractions of α and β phases for new alloys and temperatures, (ii) to calculate the effect of alloying elements and heat treatment temperature on the volume fractions of α and β phases individually as well as in combination of two or more inputs, and (iii) to estimate the effect of composition and heat treatment temperature on phase volume fractions quantitatively by calculating index of relative importance of the input parameters. As ANN models have been designed using statistical techniques, hence the results are discussed with respect to metallurgical perspective.

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2. Materials

The experimental measurements coming from the experiments conducted in house [15–18] and from the literature [19–24] belonging to seventeen titanium alloys at different quenching temperatures has been used in the present study. The larger part of the data sets in the present work are the $\alpha + \beta$ alloys; and the remaining data are near-α and single phase α alloys. In order to examine the phase volume fractions at high temperature, small sections ($20\ \mathrm{mm} \times 10\ \mathrm{mm} \times 10\ \mathrm{mm}$) of each Ti alloy were soaked at various temperatures for 30 min, followed immediately by water quenching. Each specimen was slurry coated with Deltaglaze-151 to reduce the oxidation prior to heating to the test temperature. The heat-treatment at 750, 815, 900, and 950 °C are primarily selected, because they are common $\alpha + \beta$ hot working temperatures for most of the two phase titanium alloys. The chemical compositions (Al, V, Fe, O, and N) and temperature are the inputs and the corresponding two outputs are α and β phase volume fractions. The statistics of the inputs and output parameters are presented in the Table 1. All the variables were normalized between 0.1 and 0.9. The normalization process is expressed quantitatively as follows:

$$x_n = \frac{(x - x_{\min}) \times 0.8}{(x_{\max} - x_{\min})} + 0.1$$

where x_n is the normalized value of x; $x_{\max}$ and $x_{\min}$ are the maximum and the minimum values of x, respectively, in the entire data set. Once the best-trained network was found, all the transformed data were put back into their original value by the following equation:

$$x = \frac{(x_n - 0.1)(x_{\max} - x_{\min})}{0.8} + x_{\min}$$

3. Modeling procedure

In the present study, the model was trained using a back propagation algorithm and the sigmoid function was used as an activation function [25,26]. A detailed description of the back propagation algorithm and training procedure has been reported previously [26–28]. The training program and the graphical user interface design of the present model was written in C and Java, respectively.

The model consists of six neurons (Al, V, Fe, O, N, and heat treatment temperature) in the input layer and two neurons (α and β phase volume fractions) in the output layer (see Fig. 1). The neural network training consists of adjusting the weights associated with each connection between the neurons until the computed outputs for each set of input data are as close as possible to the experimental output values. To determine the optimum architecture and to find the confidence of ANN model, the data sets split into training and testing datasets. The available 134 data sets were divided into 99 training data sets and 35 testing data sets. Appropriate

Table 1
Statistics of alloying elements, heat treatment temperature (inputs) and volume fraction of α and β (outputs) used in the present model development.

Experimental data	Input and output variables	Minimum	Maximum	Mean	Standard deviation
99 Training + 35 test data sets	Al (%)	5.72	7	6.244	0.071
	V (%)	1.5	5	3.948	0.071
	Fe (%)	0.01	3.04	0.444	0.049
	O (%)	0.08	0.3	0.148	0.016
	N (%)	0.003	0.02	0.007	0.000
	Temperature (°C)	600	1000.62	861	132.158
	α phase volume fraction (%)	0	100	52.7	42.002
	β phase volume fraction (%)	0	100	47.3	42.002

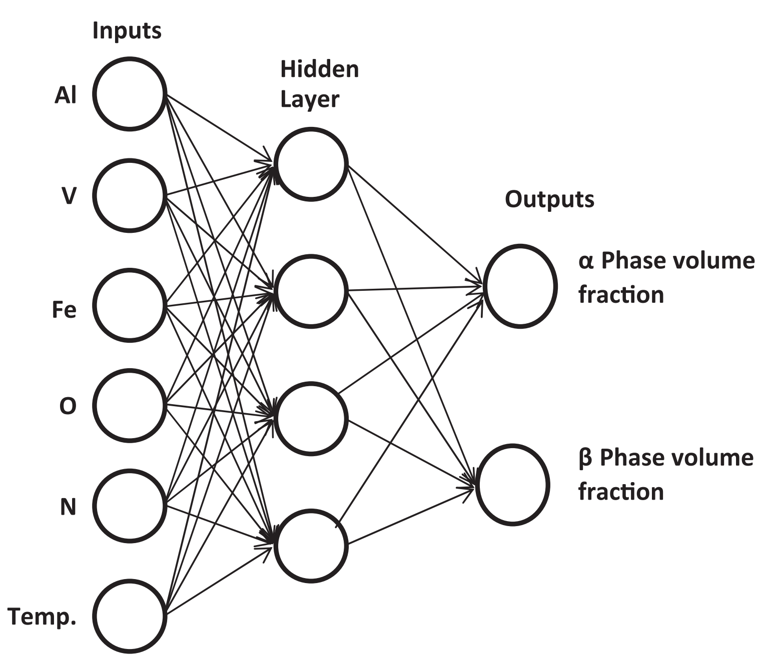

Fig. 1. Schematic diagram of neural networks model representing the hidden layers in between the inputs and respective outputs.