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Optimization of chemical composition for TC11 titanium alloy based on artificial neural network and genetic algorithm

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ABSTRACT

It is quite difficult for materials to develop the quantitative model of chemical elements and mechanical properties, because the relationship between them presents the multivariable and non-linear. In this work, the combined approach of artificial neural network (ANN) and genetic algorithm (GA) was employed to synthesize the optimum chemical composition for satisfying mechanical properties for TC11 titanium alloy based on the large amount of experimental data. The chemical elements (Al, Mo, Zr, Si, Fe, C, O, N and H) were chosen as input parameters of the ANN model, and the output parameters are mechanical properties, including ultimate tensile strength, yield strength, elongation and reduction of area. The fitness function for GA was obtained from trained ANN model. It is found that the percentage errors between experimental and predicted are all within 5%, which suggested that the ANN model has excellent generalization capability. The results strongly indicated that the proposed optimization model offers an optimal chemical composition for TC11 titanium alloy, which implies it is a novel and effective approach for optimizing materials chemical composition.

1. Introduction

Titanium and its alloys are characterized by high specific strength and excellent corrosion resistance, which are widely applied in the fields of marine [1], aeronautics [2] and biology [3]. However, with the rapid development of aerospace industry, titanium alloys are experiencing an increasing demand to obtain higher mechanical properties at room temperature and maintain reliability under elevated temperature conditions. Generally, the mechanical properties of titanium alloys not only depend on the microstructure and processing, but also are more associated with alloying elements. In order to improve the property of materials, it is extremely necessary to conduct the quantitative analysis of alloying elements contents on the basis of understanding about the influence of elements on the property. Therefore, the alloying elements contents can be designed and adjusted to meet the demand of corresponding standards. In the previous reports, some studies with regard to the relationship of alloying elements and mechanical properties have been carried out by the materials researchers. For example, Zhao et al. [4] studied the effects of the alloying element Cr on the titanium burning behavior by means of the DCSB method, which is by igniting titanium for a certain time under certain direct current. It was found the fact that the burning velocity of titanium alloys decreases if the Cr content is larger than 10%. Sutou et al. [5] researched the effect of alloying elements on the *Ms.* temperature, ductility and the shape memory properties of Cu–Al–Mn ductile shape memory alloys with the help of differential scanning calorimeter, cold-rolling and tensile test techniques. The author suggested that the *Ms.* temperature in Cu_{73}–Al_{17}–Mn_{10} (at.%) ternary alloy increased by adding Zn, Au and Si, and decreased by adding Ti, Cr, Fe, Co, Ni, Ag and Sn. Jiang et al. [6] studied the influence of alloying elements on mechanical properties and microstructures of sintered Nd–Fe–Co–B magnet using optical microscopy, SEM and EDX. The maximum bending strength is obtained in the Nd–Fe–Co–B magnet with 0.5 at.% Cu or Nb when the sintering is conducted at 1060 °C. Unfortunately, the research work mentioned above mainly focused on the traditional experimental method to study the relationship between alloying elements and mechanical property of metal materials. But many factors affect the property, and the effects of these factors on the property present complicated and highly non-linear relationship. Hence, it is quite difficult to develop the accurate relation model using experimental and mathematical approach.

The TC11 alloy, as a kind of $\alpha + \beta$ type heat resistance titanium alloy, is an excellent candidate for aerospace applications because of its good thermo-stability and corrosion resistance, high strength to weight ratio, and higher servicing temperature of 500 °C, which makes it a desired material in aero engine blades, compressor disks

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and other crucial components in airplanes [7,8]. Some researches about this alloy have been reported previously, including hot deformation behavior [9], microstructrual globalization mechanism [10], flow softening and microstructrual evolution [8]. However, the optimization of alloying elements is quite complex because there is significant effect of alloying elements on the mechanical properties, which suggests that it is crucial to control the suitable elements content in order to obtain the high property materials before deformation. As a result, it is of great importance and benefit to study the influence of alloying elements on the mechanical properties and establish their optimization model. In the practical operations, optimum condition of alloying elements to achieve the best property is often designed from references or handbooks, and then adjusted subsequently by a trial-and-error method, which is costly and time consuming, as well as highly dependent on the experience of the materials researchers.

In the recent years, with the help of artificial intelligent technology, soft computing method is extensively used in the field of materials science to predict property and optimize processing. As the branch of artificial intelligence, artificial neural network (ANN) has become a practical and powerful tool to model complex non-linear systems [11–15], and genetic algorithm (GA) also can be found in various research fields for parameter optimization [16–18]. In addition, both techniques are considered to be appropriate in the process optimization, and researchers began to optimize process to attain excellent properties using ANN and GA. In the present investigation, based on the large amount of experimental data of TC11 titanium alloy, the chemical composition optimization model that leads to the ideal mechanical properties has been developed using the combined approach of ANN and GA. An optimal setting of chemical composition for TC11 titanium alloy can be obtained by solving the optimization problem.

2. Theory of artificial neural network and genetic algorithm

Artificial neural network (ANN) is generally accepted as a technology offering an alternative way to simulate ambiguous and complex problems. It has the capability to transform a non-linear mathematical model into a simplified black-box structure. The advantages of using neural networks in process modeling are that they have learning and generalization abilities as well as nonlinearity. Numerous applications of ANN have been realized in pattern recognition, materials modeling, data analysis and property prediction [19–22]. A neural network is a computational structure, consisting of a number of highly interconnected processing units called neurons. The neurons are connected to each other by weighted links over which signals can pass. Each neuron receives multiple inputs from other neurons in proportion to their connection weights and generates a single output, which may be propagated to several other neurons [23]. Among diverse types of ANN models, back-propagation (BP) algorithm, an iterative gradient algorithm, is so popular that it has been used for the present work. BP neural network consists of an input layer, one or more hidden layers and an output layer, but most pattern recognition and classification tasks can be completed with single-hidden layer, which is shown in the Fig. 1. BP neural network possesses hierarchical feed forward network structure, the outputs of each layer are directly sent to each neuron in the next layer. Suppose each input neuron is represented by its value x. Each connection between the neurons is characterized by its weight w. The value of a neuron is multiplied by the corresponding weight and added to the value of the signal in the neuron of the next layer to produce a single output (y). In addition, the value of bias neuron or threshold θ is added to the equation

$$y = f\left(\sum wx + \theta\right) \tag{1}$$

The activation function f is usually the sigmoid function, which makes the modeling of an arbitrary continuous non-linear relation between input and output variables. The sigmoid function can be mathematically expressed as

$$f(x) = \frac{1}{1 + \exp(-x)} \tag{2}$$

A series of known input and output data sets are used to let the neural network learn the internal relationship in the data set by adjusting the weight w and thresholds θ gradually. The learning procedure of network is considered completed until the mean squared error (MSE) reaches a minimum value, which is described as

$$MSE = \frac{1}{n}\sum_{j=1}^{n}[y_j^d - y_j^o]^2 \tag{3}$$

where y^d is the desired response and y^o is the output response from ANN, and n is the patterns presented. Such process of minimize the mean squared error is called as training the network. After the training the network, the weights network are saved in order to predict outputs corresponding to a given input.

Genetic algorithm (GA) is one of classic population-based robust search and global optimization methods, which is developed by John Holland and his colleagues at the University of Michigan [24]. Based on the mechanics of natural selection and evolution, the algorithm solves optimization problems imitating nature in the way it has been working on the evolution of life for millions of years. The GA is different from most optimization techniques because of their global searching from one population of solutions rather than from one single solution. It can deal with linear and non-linear problems by exploring all regions of the state space and exploiting promising areas through mutation, crossover, and selection operations applied to individuals in the population. Fig. 2 is schematic view of a genetic algorithm. As shown in the Fig. 2, each individual in a population is represented by a chromosome. After initialization of the first generation, the fitness of each individual is evaluated by an objective function. In the reproduction step, the genetic operators of parent selection, crossover and mutation are applied, thereby providing the first offspring generation. Iteration is performed until the objective function converges.

3. Modeling of chemical composition optimization using ANN and GA approach

3.1. ANN model for property prediction of TC11 titanium alloy

The complex relationship between alloying elements and mechanical properties of TC11 titanium alloy cannot be described by traditional modeling approach accurately. While it is appropriate for ANN technique to model the property prediction, and thus is employed as modeling tool in the present investigation. Collection and analysis of a reliable database is the first critical step since the performance of an ANN model depends on the dataset used for training. The data used for the ANN model is collected from the forging and tensile tests of TC11 titanium alloys, which were prepared with the shape of round cake, under the same condition of hot processing, including heat number, batch code, forging style and heat treating. Forging test was conducted on the 25T-M counter-blow hammer. Tensile test was carried out on Zwick/Z150 universal testing machine at room temperature and initial tensile rate of 0.6 mm/min. Because mechanical property of this alloy is quite sensitive to its alloying elements, the input for the present model is the chemical composition of TC11 titanium alloy, whereas