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Modeling effects of alloying elements and heat treatment parameters on mechanical properties of hot die steel with back-propagation artificial neural network

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ABSTRACT

Materials data deep-excavation is very important in materials genome exploration. In order to carry out materials data deep-excavation in hot die steels and obtain the relationships among alloying elements, heat treatment parameters and materials properties, a 11×12×12×4 back-propagation (BP) artificial neural network (ANN) was set up. Alloying element contents, quenching and tempering temperatures were selected as input; hardness, tensile and yield strength were set as output parameters. The ANN shows a high fitting precision. The effects of alloying elements and heat treatment parameters on the properties of hot die steel were studied using this model. The results indicate that high temperature hardness increases with increasing alloying element content of C, Si, Mo, W, Ni, V and Cr to a maximum value and decreases with further increase in alloying element content. The ANN also predicts that the high temperature hardness will decrease with increasing quenching temperature, and possess an optimal value with increasing tempering temperature. This model provides a new tool for novel hot die steel design.

1. Introduction

Materials genome technologies, which have been developed recently, are believed to change traditional means of materials design. Materials data deep-excavation is one of the key technologies in materials genome technologies[1-7]. It is also established that artificial intelligent methods can carry out materials data deep-excavation efficiently[8,9]. As an artificial intelligent method, artificial neural network (ANN) has self-teaching capabilities and can be used as a computational mode designed to mimic human brain architecture and operations. ANN can construct mathematical models from experiment data and has shown remarkable performance when used to model complex linear and nonlinear relationships in materials science and engineering recently, especially in handling multivariable problems without regularity[10,11]. For instance, Huang et al.[12] investigated the mechanical properties of ceramic materials using artificial neural network. Col et al.[13] successfully predicted the toughness of micro-alloyed steel based on industrial production conditions using this method. Sitek et al.[14] proposed a methodology employing neural networks that can model the relationships among high-speed steels properties, chemical composition and heat-treatment parameters. Li et al.[15] applied an artificial neural network to acquire the effects of deformation technological parameters on the mechanical properties of TC11 alloy. You et al.[16] developed a new artificial neural network model to optimize the content of carbon in low-alloy engineering steels.

Hot die steel shows excellent temperature resistance, and has been widely applied in fabrication, aviation, aerospace and related metallurgy industries[17-19]. The high temperature resistance is attributed to its alloying elements, such as Cr, Ni, Mn, V, Si, Nb, and W; each of such element has a positive impact on mechanical properties. Investigations have been carried out on the relationships between mechanical properties and constituent elements for hot die steel. Most of these studies are experimental and qualitative[20,21], and no mathematical model

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has been reported on the effects of alloying elements on the mechanical properties due to the complexity in formulating such models. However, it is well known that such mathematical model is of critical importance to design new hot die steel.

The abilities of ANN to learn complex relationships between input and output parameters and to allow user to examine the effect of each parameter on the properties of hot die steel make it a significant analytical tool. The mathematical models relating chemical compositions to material properties obtained by ANN would greatly facilitate the novel design of different kinds of steels. To date, such relevant research has rarely been reported. In this paper, an artificial intelligent model was constructed, followed by artificial neural network training and verification; and the effects of alloying elements and heat treatment parameters (quenching and tempering temperatures) on materials properties for hot die steel were obtained using this artificial neural network.

2. Modeling and Algorithm

In present study, multi-layered feed-forward back-propagation (BP) algorithm was selected. This algorithm is currently one of the most common supervised learning algorithms. Supervised learning implies that a good set of data or patterns is needed to train the network. Input-output pairs are presented to the network and weights are adjusted to minimize the error between network output and actual values. The knowledge of neural network is stored in these weights. Back-propagation training algorithm is an iterative gradient algorithm, which is designed to minimize the mean-squared error between the predicted and desired output values. A back-propagation model consists of an input layer, some hidden layers and an output layer.

2.1. Architecture of BP artificial neural network

Modeling the relationships among chemical compositions, heat treatment technologies and mechanical properties is important for designing a novel alloy. However, rarely precise model has been built to clarify these relationships for hot die steel. Due to its advantages, BP ANN was selected to model these relationships. Considering the complexity and limited data, two hidden layers were selected. Since mechanical properties are determined by chemical compositions and heat treatment technologies for hot die steel, 11 neurons in input layer and 4 neurons in output layer were determined. The neurons in the input layer denote the 9 alloying elements (C, Cr, Ni, Mo, Mn, Si, V, W, and Mn) and two heat treatment variables (quenching and tempering temperatures). The neurons in the output layer denote high temperature hardness, room temperature hardness, tensile strength and yield strength, respectively.

For BP network, an experimental formula can be used to determine the number of neurons in hidden layer:

$$n_1=(m+q)^{0.5}+s \quad 0\leqslant s\leqslant 10 \tag{1}$$

where, q, m and n_1 are the numbers of neurons in input, output and hidden layer, respectively. According to this equation, it was determined that $n_1\leqslant 14$. Furthermore, the number of neurons in hidden layer was optimized by testing network performance with various values of neurons number. Finally, a $11\times 12\times 12\times 4$ network was determined. The network architecture is shown in Fig. 1.

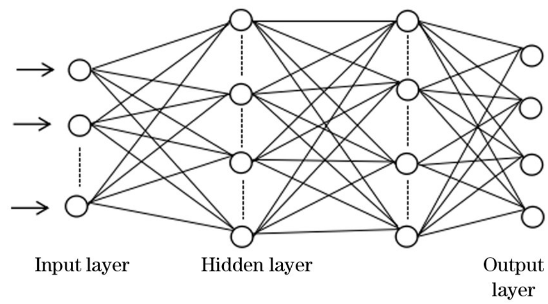

Fig. 1. Architecture of network with $11\times 12\times 12\times 4$.

2.2. Algorithm of training back-propagation network

The flow chart of back-propagation algorithm is illustrated in Fig. 2.

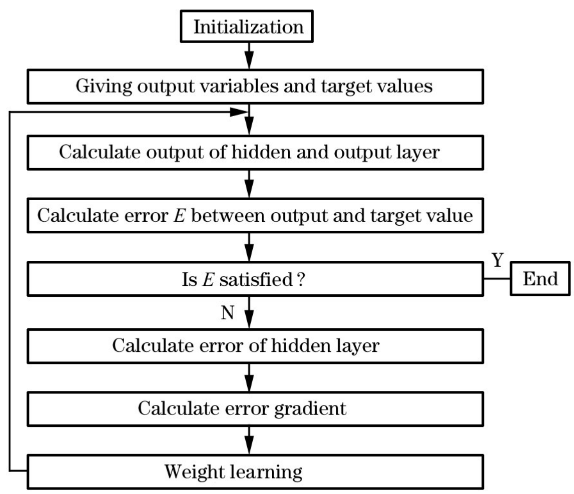

Fig. 2. Flow chart of BP ANN algorithm.

It is assumed that there are s neurons in input layer, m neurons in the first hidden layer, n neurons in the second hidden layers, and q neurons in output layer. The inputs of input layer are P_1, P_2, P_3, $\cdots$, P_i. W_{ij} is the connecting weight between the ith neuron in one layer and the jth neuron in the subsequent neighbor layer, b is the threshold value of hidden layer, and $f(x)$ is a logistic sigmoidal ac-