Modeling on Mechanical Properties of Zr-4 alloy Special Pipe during Annealing Treatments by ANN

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Abstract. In this paper, the influence of Annealing treatments and deformation on the mechanical properties of Zr-4 special pipe were modeled by artificial neural network (ANN). the optimal network architecture was considered to be 3-6-6 with momentum factor is 0.8 has been developed. The influence between mechanical properties of Zr-4 special pipe under different Annealing treatments and deformation has been proposed by using ANN model. It shows that the RMSE is 2.632, which shows good performance and results. The yield strength and tensile strength is slow dawn at first and then rise smoothly by reducing the second annealing temperature at room temperature. the elongation is going up and dropping with reducing the second annealing temperature at room temperature. The Part1 needed to cause recrystallization.

1. Introduction

Zirconium alloys are now being increasingly used for nuclear industry and still have the potential materials for the next-generation nuclear reactor, because of its low thermal neutron capture cross section, desirable corrosion resistance and favorable mechanical properties at high temperature about 300−400°C. Zr-4 special pipe is an important structure of the nuclear power reactors, which has been mainly taken control rod for supporting, guidance and cushion. It is a poor mechanical property of Zr-4 special pipe may cause control rod lifting and lowering action, which is danger for the nuclear power reactor [1-3]. In recent years, many important researchers have already studied in detail the effects of mechanical properties of Zr-4 alloys on annealing treatment. The Zirconium alloys are completely softening after 8minutes at 650°C, 1 minute at 750, and 1/4 minute at 800°C. From approximately 100-150°C, there was an 11% decrease in resistivity. There was no accompanying change in hardness, microstructure or in preferred orientation. Bostrom and Kulin found a continuously increasing activation energy as the fraction of electrical resistivity change increased [4]. Zhao Xicheng et.al studied the effects of annealing temperature on microstructure and properties of Zr-4 processed by surface mechanical attrition treatment, and found that the surface microhardness of Zr-4 decreases obviously due to grain growth during the process of recrystallization at 350°C of annealing temperature [5]. But it is still seldom literatures were published for mechanical properties on annealing treatment and deformation in the case of Zr-4 special pipe. Therefore, the main objective of the present
work is to focus on the influence of Annealing treatments and deformation on the mechanical properties of Zr-4 special pipe.

Most of studies on the effect between mechanical properties and heat treatment parameters for this alloy have been accomplished by some trial and error testing method, which depends considerably on the designer's skill and experiences. In this paper, the influence of Annealing treatments and deformation on the mechanical properties of Zr-4 special pipe were modeled by artificial neural network (ANN). ANN is a non-linear algorithm which is used for modeling of process parameters, but cannot find optimum condition and may be hampered in the local minimum and overfitting the results indicated that ANN model is an efficiently tool to evaluate and predict the mechanical properties of Zr-4 special pipe under different Annealing treatments and deformation.

2. Methodology

2.1. Network structure

An ANN is a mathematical model consisting of a number of highly interconnected processing elements organized into layers, the geometry and functionality of which have been likened to that of the human brain. ANN learns by experience, generalize from previous experiences to new ones, and can predictions where the result is not known. In ANN, the layer that receives inputs is called the input layer, and that which gives the output (or output vector) is called the output layer. Other layers, as they do not receive any direct input or contribute to output directly, are called hidden layers. A standard network structure is composed of an input layer, one hidden layer (one or more hidden units) and one output layer. Each layer consists of many units or 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. In each layer, units receive their input from the preceding layer's units and send their output to units in the subsequent layer. The configuration of layers in a neural network is called network structure. Hornik et al. [12] have shown that an ANN with one hidden layer with sigmoid (logarithm sigmoid or hyperbolic tangent) activation function can map any function of practical interest. Fig.1 shows a schematic representation of the neural network architecture used in this study [6]. The input layer and the output layer consist of all the input factors and target vectors, respectively. The number of hidden units in hidden layer affects the generalization capability of the network. For smaller number of hidden units, the ANN may not be adequate, whereas with too many hidden units may have the risk of overfitting the training data and poor generalization on the new data.

Fig.1 The structure of BP neural network
2.2. Network training and testing

In neural networks, the training process is used to learn patterns present between network inputs and target outputs after the network weights and biases have been initialized by means of a training algorithm. The objective of training is to find the set of weights and biases between the neurons that determines the global minimum of error function. This process is equivalent to fitting the neural network model to the available training data. Normally, training the network with an appropriate method is the key factor in order to get a well-trained network. If the network is properly trained, it has then learned to model the function that relates the input variables to the output variables and can subsequently be used to make predictions where the output is not known. This process is called testing and the ability of this network is called generalization [7-9].

3. Experimental

The composition of Zr-4 special pipe material, used in the present study, is following (in wt%): 1.2~1.7Sn, 0.18~0.24Fe, 0.07~0.13Cr, ≤0.027 C, ≤0.0025 H, ≤0.16O, Fe balance. The formation of Zr-4 special pipe shows in Fig 1. The first and second Annealing treatments are used by vacuum annealing furnace in NWZ. The Annealing temperature for sample presented in Table 1. The mechanical properties were test for part1 and part2 based on GB/T228.1-2010. The individual grains were obtained by using the leica DM2500M optical microscope.

The alloys employed in this study have been published by YangIl Jung, et.al [8]. The total data based on experiments was considered for analysis, which were divided into two groups, 300 data sets for the training and 80 data sets for the testing. chemical compositions, annealing temperature and annealing time as input data were normalized in the range of -1 to 1 using E.q (1) while hardness as output date were normalized in the range of 0 to 1 using E.q (2), respectively [9].

\[ X_{\text{normalized}} = \frac{2}{X_{\text{max}} - X_{\text{min}}} (X - X_{\text{min}}) - 1 \]  

\[ Y_{\text{normalized}} = \frac{Y - Y_{\text{min}}}{Y_{\text{max}} - Y_{\text{min}}} \]

where \( X_{\text{normalized}} \) is the normalized value of the input units X (annealing temperature, annealing time and deformation); \( X_{\text{max}} \) and \( X_{\text{min}} \) are the maximum and minimum values of X respectively; \( Y_{\text{normalized}} \) is the normalized value of the output unit (yield strength, tensile strength and elongation); \( Y_{\text{max}} \) and \( Y_{\text{min}} \) are the maximum and minimum values of Y respectively.

| No. | 1st Annealing Temperature/ °C | 2nd Annealing Temperature/ °C |
|-----|-----------------------------|-----------------------------|
| 1   | 555                         | 500                         |
| 2   | 555                         | 523                         |
| 3   | 540                         | 523                         |
| 4   | 523                         | 523                         |
4. Results and discussion

4.1. Variation parameters on model

The performance of the ANN depends on the network parameters such as numbers of neurons in the hidden layer and momentum factor \(^{[10]}\). In the present work, a standard feed-forward network with one hidden layer was employed. The optimal number of units in the hidden layer was determined by the try and error procedure. The range of hinder units can be determined by Eq. (3):

\[ N_H = \sqrt{N_{in} + N_{out} + a} \]

(3)

Where \( N_H \) is the number of units in the hinder layer in the try and error procedure, \( N_{in} \) is the number of units in input layer, \( N_{out} \) is the number of units in output layer, and \( a \) is the parameter in the range 1 to10\(^{[9]}\). Therefore, the number of units in the hidden was examined from 2 to 12. Fig.3a shows the Root mean square error (RMSE) for both training for various numbers of units in the hidden layer by Eq. (4), where \( T_i \) is the target output and \( Y_i \) is the network output, respectively. It is evident that the network with 6 hidden units has the smallest error for testing data. The effects of momentum factor on the performance of the developed ANN are shown in Figs. 3(b), which the RESE is 2.632. As can be seen, the optimum values of momentum factor are 0.8. Therefore, the network with 8 units in the hidden layer was used in this work and the optimal network architecture was considered to be 3-6-6, and the optimum values of momentum factor and learning rate is 0.8.

\[ RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (T_i - Y_i)^2} \]

(4)

![Fig.3 Variation of sum square error with parameters](image)

(a) Hidden units (b) Momentum factor

4.2. Effect of Annealing treatments on mechanical properties

The effect of annealing temperature on mechanical properties at room temperature have been presented in Fig 4 for Zr-4 alloy special pipe at various deformation. As can be seen from the Fig 4(a) and (b), the deformation of Part1 is 50% while the first annealing temperature is beginning at 555 and dropping slowly at 523 \(^{\circ}C\), so the yield strength and tensile strength is slow dawn at first and then rise smoothly at room temperature. However, the elongation is going up and dropping with reducing the second annealing temperature at room temperature.
Fig. 4 Effect of annealing temperature on mechanical properties at room temperature on the Zr-4 alloy special pipe

4.3. Effect of Annealing treatments on metallographic structure

The optical microstructures for various schemes with different deformation can be seen in Fig 5 and 6. As we can show in Fig 5 that there is not clean on the grain boundary for Part 2 (19%), which is called un-recrystallization. However, Part 1 (50%) shows that the recrystallization, because there is clean on the grain boundary at Fig 6. At first, a strain-free nucleus is formed when one of existing grain boundaries move into its neighbor, leaving a strain-free recrystallized region behind. The boundary moves into the grain which contains the higher dislocation density in the local region. In the second nucleation new grain boundaries are formed in regions of sharp lattice curvature through subgrain growth. This mechanism sees to predominate at high strains, with nuclei appearing at grain boundaries, twin boundaries, or at inclusions or second-phase particles. The minimum amount of deformation is greater than 20%, what part 1 is 50% and Part 2 is 18%. So, the Part 1 needed to cause recrystallization while Part 2 is un-recrystallization. Increasing the annealing time and temperature may decrease the recrystallization.

Fig. 5 The Optical microstructures of the deformation 18 (Part 2) for various schemes

![Image](image1.png)

(a)scheme 1       (b)scheme 2          (c)scheme 3         (d)scheme 4

Fig. 6 The Optical microstructures of the deformation 50 (Part 1) for various schemes

![Image](image2.png)

(a)scheme 1       (b)scheme 2          (c)scheme 3         (d)scheme 4
5. Conclusion
(1) The influence between mechanical properties of Zr-4 special pipe under different Annealing treatments and deformation has been proposed by using ANN model. It shows that the RMSE is 2.632, which shows good performance and results.
(2) In this paper, the optimal network architecture was considered to be 3-6-12 with momentum factor is 0.8 has been developed.
(3) The yield strength and tensile strength is slow dawn at first and then rise smoothly by reducing the second annealing temperature at room temperature. However, the elongation is going up and dropping with reducing the second annealing temperature at room temperature. It is indicated that the yield strength and tensile strength of Part1(50% deformation) is much lower than the Part 2(18% deformation), and the elongation of Part1(50% deformation) is much higher than the Part 2(18% deformation).
(4) The Part1 needed to cause recystallization while Part 2 is un-recystallization.

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