Exploring Microstructure Evolution and Machine-learning Method During Hot Deformation of 56Ni-32Ti-12Hf Alloy

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Abstract: Hot compression simulation tests were carried out on a 56Ni-32Ti-12Hf alloy at temperatures ranging from 800 to 1000 °C and strain rates ranging from 0.001 to 1 s^{-1}. The study aimed to explore the hot deformation behavior and microstructure evolution mechanism of the alloy. A flow stress prediction models was developed: a chaotic mapping adaptive inertia weight whale optimization algorithm-optimized back propagation neural network (CIWOA-BPNN) model based on machine learning. The hot processing map of the 56Ni-32Ti-12Hf alloy was developed using dynamic material modeling (DMM) theory and flow stress data predicted by the CIWOA-BPNN model. The optimal hot processing range was found to be between temperatures of 875–975 ℃ and strain rates of 0.001–1 s^{-1}. The study found that within the optimal processing interval, the softening mechanisms observed were discontinuous dynamic recrystallization (DDRX) and continuous dynamic recrystallization (CDRX).

Keywords: Machine learning; NiTiHf alloys; Constitutive model; CIWOA-BP algorithm

1 Introduction

NiTi shape memory alloys are vital functional materials used in various industries such as aerospace (e.g., turbojet nozzles) [1], space communications (e.g., antennas) [2], biomedicine (e.g., brackets) [3], and fluid transmission (e.g., actuators) [4]. Specifically, NiTiHf alloys are known for their high hardness and yield strength. However, due to the limited plasticity, its processing is a challenge [5, 6]. Additionally, the variation law of flow stress with deformation parameters (e.g., strain, strain rate, and temperature) during hot deformation of alloys has been of great interest [7]. The processing of NiTiHf alloys presents challenges, and its microstructure and properties are highly sensitive to deformation parameters [5, 6]. Furthermore, the hot deformation mechanism and constitutive relationship of NiTiHf ternary alloy remain unclear. This paper aims to address these research gaps by utilizing 56Ni-32Ti-12Hf (wt.%) alloy as the experimental material. Through hot simulation experiments, true stress-strain data was obtained and used to develop a CIWOA-BPNN model. The CIWOA-BPNN model was to verify its accuracy. Subsequently, the hot processing of the alloy was mapped based on the data predicted by the CIWOA-BPNN model. Finally, the microstructure after hot deformation was analyzed to validate the reliability of the hot processing map. A model based on an improved machine learning algorithm for predicting the flow stress is proposed in this work. It also provides a theoretical guide for the selection of process parameters for the hot processing of NiTiHf alloys.

2 Experimental procedure

The nominal composition of 56Ni-32Ti-12Hf (wt.%) alloy was prepared by vacuum-induction melting. The hot compression test was implemented through the Gleeble 3800D hot simulation testing machine. After the thermal compression test, the samples were cut from the middle along the axis by wire cutting. The obtained samples were inlaid, ground, polished, and corroded. Then, Zeiss optical microscope (OM) and a scanning electron microscope (SEM) equipped with electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM) were used for microstructure observation and analysis.

3 Result and discussion

1 Modeling of flow behavior

To ensure the flow stress prediction accuracy remains unaffected by the model structure, Liu et al. [8] adopted a backpropagation neural network model. This method is more apt for handling intricate and fluctuating data, accurately forecasting the material’s flow stress during hot deformation. This study adopts a three-layer neural network with a single hidden layer, as depicted in Fig. 1. The structure of Fig. 1 shows the weights and thresholds between layers, which directly determine the learning effect of the prediction model. However, the traditional BP neural network model recognizes the samples to be tested mainly through the back-propagation algorithm and gradient descent method to optimize the network’s weights and thresholds. Therefore, in this paper, the optimization method of the BP neural network weights and thresholds search using the optimized WOA algorithm (CIWOA) is to regard each neural network as an individual. Fig. 2 illustrates the correlation between the training values in the CIWOA-BPNN model's network output. It demonstrates the accurate capture of the connection between input and output, as evidenced by a high correlation coefficient of 0.99812. Consequently, the CIWOA-BPNN model exhibits effective predictive capability for the flow stress of the 56Ni-32Ti-12Hf alloy.

2 Establishment of the processing map

By substituting the predicted value by the CIWOA-BPNN model into Eq. (1), the instability coefficient contours maps of the 56Ni-32Ti-12Hf alloy at true strains of 0.1 and 0.7 are produced, as illustrated in Fig.3a and 3b. The instability region mainly appears under high $\dot{\varepsilon}$ value conditions, with the area of the instability region increasing with the increase of strain. A hot processing map based on the CIWOA-BPNN model of 56Ni-32Ti-12Hf with a strain of 0.7 is obtained by superimposing Fig. 3a and 3b, as shown in Fig. 4. In this representation, the gray part represents the instability regions (T = 825–875 ℃, $\dot{\varepsilon}$ = 0.5–1 s^{-1}; T = 925–1000 ℃ and $\dot{\varepsilon}$= 0.5–1 s^{-1}).

3 Deformation mechanism

To explain the softening mechanism of, the deformed microstructure was observed by EBSD. Local misorientations (point-to-point) and cumulative misorientations (point-to-origin) of the two deformed grains extracted from Fig. 5a and 5b are analyzed, respectively. Measurement lines are drawn along the compression direction and vertical directions (Fig. 5). It can be observed that the misorientation accumulated along GBs and inside GBs exceeds 10° in both compression and vertical directions. This indicates that the migration and accumulation of dislocations leads to the gradual rotation of sub-grain boundaries into high-angle grain boundaries (HAGB). The sub-grain boundary orientation angle of B_2 is 12.1° (Fig. 5b), which falls within the medium angle grain boundary (MAGB) range of 10°–15°. Therefore, it is easier to transform into a HAGB [9]. Both phenomena are typical of CDRX [10, 11].

4 Conclusion

(1) The true stress-strain curve of 56Ni-32Ti-12Hf alloy exhibits obvious DRX softening characteristics. The peak stress rises with increasing strain rate or decreasing deformation temperature.

(2) The CIWOA-BPNN model has higher accuracy in predicting the high-temperature flow behavior of 56Ni-32Ti-12Hf alloy.

(3) The optimal processing parameters for the 56Ni-32Ti-12Hf alloy are also determined as a hot deformation temperature range of 875–975 °C and a strain rate range of 0.001–1 s^{-1}.

(4) The softening mechanisms of the alloy in the optimal processing interval are DDRX and CDRX within the optimal machining interval determined.

Acknowledgments

This work was supported the Liaoning Provincial Natural Science Foundation Joint Fund-Doctoral Research Initiation Program(2023-BSBA-258), Project of Liaoning Provincial Department of Education(JYTMS20231200).

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