

Thermomechanical Process Modelling of 40NICRMO8-4 Alloy by Artificial Neural Networks

(Model Proses Termomekanikal Bagi Aloi Jenis 40NICRMO8-4 Menggunakan Rangkaian Neural Buatan)

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ABSTRACT

Artificial neural networks (ANNs) as simplified model of mankind's neural system, are capable of simulating and predicting real world complex problems which are challenging and expensive to model physically. In this study the correlation between the flow stresses and strain rate, temperature, strain in thermomechanical process of 40NICRMO8-4 alloy has been modelled. The results revealed that flow stress for every strain value is less at high temperatures compared to those at low temperatures and material resistance against deformation will also decrease as temperature goes down. Moreover, increasing in strain rate when temperature is constant results in recrystallization to happen in higher strain values at times shorter. The employed neural network for this study was a feed forward multilayer perceptron trained with common back propagation algorithm. Similar to any other ANNs, the employed network receives some parameters as inputs and delivers some as outputs. The inputs given to this model were temperature, strain and strain rate while flow stress parameter was collected as requested output. Outputs, with high precision of approximately 99% accuracy, were predicted and produced during training phase. Likewise, the predicted output of the ANN model achieved an R-value of about 0.99871 compared with of those experimental values. Best results were obtained with an ANN model consist of two hidden layers trained with Levenberg–Marquardt training algorithm.

Keywords: Thermomechanical Process; 40NICRMO8-4 Alloy; Artificial Neural Network; Flow Stress

INTRODUCTION

40NICRMO8-4 alloy steel is a heat treatable and low alloy steel containing chromium, nickel and molybdenum. It has high toughness and strength in the heat treated condition. AISI 4340 alloy steel is mainly used in power transmission gears and shafts, aircraft landing gear, and other structural parts. This steel has better penetration of quench than 39CrNiMo3 which is used for components with a lot of stresses such as shafts, axles, engineering nut and fasteners, etc. The dynamic deformation characteristics of many steels have been intensively studied for military or engineering applications in recent decades. In order to do thermomechanical process in steels, it is necessary to control parameters such as temperature, strain rate in hot deformation processes. In this process, mechanisms such as work hardening (WH), Dynamic recovery (DRV), Dynamic recrystallization (DRX) will be occurred simultaneously (Sanrutsadakorn et al. 2013; Kim et al. 2001; Yang et al. 2017; Rajabi 2018). When hot deformation is started, dislocation density will gradually increase. The rise in deformation amount will lead to dislocation density increase, climbing and cross

slip dislocation. As a result, Polygonization Mechanism or dynamical recovery process will happen. When the strain reaches a critical point, new grains will be nucleate by bulging and in this stage, DRX will happen. Hence, the higher strain amount, the lower flow stress will be and it will lead to steady state. At this moment, a kind of balance between their dislocation producing and their deletion will be created by nucleation process (Wang et al. 2005).

Restoration mechanism is a function of deformation conditions i.e. temperature and strain rate in hot deformation process. Consequently, from one hand, temperature can influence on atom's diffusion coefficient, ease of movement, dislocation neutralization and sub grain boundary formation and on the other hand, it can also be effective on nucleation mechanism and dynamic recrystallization growth (Beladi et al. 2017). It can be added that strain rate parameter is effective on how restoration mechanism will take place. In lower strain rates, when temperature is constant since there is enough time to do micro structural changes in restoration process, a decrease in flow stress will be observed. Generally speaking, strain rate amount can influence on both dynamical recovery process resulted from dislocation movement and

also recrystallization kinetic resulted from grain boundary movements (Drobnjak et al. 1997; Liu et al. 2000; Zhou et al. 2017).

With current fast-paced technology advancements as well as emerging of powerful mathematical models, nowadays, artificial neural networks (ANNs) as simplified models of human brain activity are able to handle complex problems. Furthermore, ANNs are capable of learning and that is what makes them unique. They utilize highly interconnected elements called neurons giving the system the ability to solve some specific complex problems which other systems are unable to solve them. Prediction, classification and pattern recognition are the most common applications where ANNs are used. In an artificial neural network every member is connected to some of the neurons of its vicinity with varying coefficients called weights (Bahrami et al. 2005). There exist various architectures for ANNs and also several types of learning algorithms to train the network with. One of the most common and prevailing architectures is feed-forward network with back-propagation learning method (Lin et al. 2009; Reddy et al. 2005). After deciding on the architecture of the network, it is time to clarify inputs and outputs of the network. In fact, the number of units in input and output layers are defined based on the study parameters. There are also some layers in between input and output layers called hidden layers. Moreover, there exist certain number of units, or so-called nodes, in each layer as the main units of ANNs (Rajabi et al. 2012). Figure 1 is just a general demonstration of a typical feed-forward ANN employing back-propagation learning method.

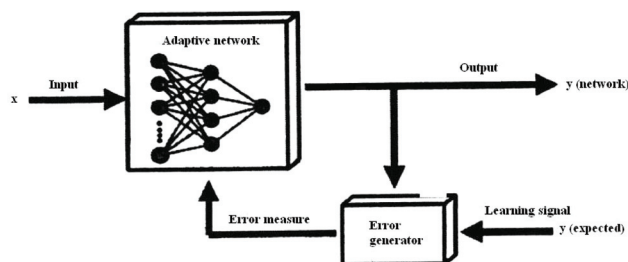


FIGURE 1. Schematic structure of the back-propagation neural network (Russell and Norving 2016)

Theoretically, there is a relationship between the number of nodes in each layer and the performance of the network in solving complex problems. Theory says, the higher the number of nodes, the less will be the error. But, it is also necessary to make a trade-off between the number of

processing units and the accuracy and processing time. In back-propagation structure, after giving the values to the input layer and after the completion of forward propagation, the error-correction step is applied. In prediction applications, the output values delivered by the output neurons of the network are compared to those targeted values of training set and these differences lead to some error values. Consequently, these error values are used to re-adjust output neuron weights in order to achieve more accurate results. Likewise, the weights of neurons located in last hidden layer are also altered in favor of getting better results. This process of re-adjusting weights spread through the network until affecting the first hidden layer neurons. That is the reason for naming such an algorithm as back-propagation. As it is necessary to have some output samples as targeted values in order to calculate the errors and provide the required feedback, this method is grouped under supervised learning methods. The concept as it was presented is pretty easy and straightforward. Since the desired outputs are available in supervised learning, the neuron weights are set after each step just to degrade the occurred error and reach the required error level (Hassoun 1995; Malinov and Sha 2003).

Artificial neural networks have drawn lots of attention recently, especially in science and engineering fields. Material science was not an exception to this (Dehghani and Nekahi, 2010; Liu et al. 2013; Rashidi et al. 2009; Reddy et al. 2009; Yang et al. 2012; Yazdanmehr et al. 2009). This study, in turn, focuses on prediction of flow stresses of 40NICRMO8-4 alloy with the help of ANNs. As it was discussed earlier, this kind of ANNs need some inputs and some target outputs. Therefore, some of the properties are given to this network as inputs and the developed network figures out the relationship between these inputs and the targeted outputs. It is notable that in all of the employed neural networks of this study, sigmoid function was chosen as an activation function in the training process.

EXPERIMENTAL APPROACH

EXPERIMENTAL PROCEDURE

The steel used in this study was 40NICRMO8-4 alloy, produced in alloy steel Esfahan complex based on chemical analysis as shown in Table 1.

In this study, the thermomechanical process tests of 40NICRMO8-4 alloy steel were carried out at the temperatures from 1173 to 1373 K and strain rates from 0.01 to 1 s⁻¹ on a dilatometer simulation machine.

TABLE 1. Chemical composition of 40NICRMO8-4 alloy steel

%C	%Si	%Mn	%P	%S	%Cr	%Mo	%Ni	%V	%Al	%W
0.39	0.295	0.73	0.005	0.004	0.82	0.26	1.85	0.01	0.015	0.02

Firstly, discs with 1cm in thickness from forged barreled ingot that has been identified without any fault in macroscopically studies has been cut and in radius direction with values in the range of 1/3-2/3 (cm) radius, dilatometer specimens with 5 mm inn diameter and 7.5 mm in height was prepared. Reaction of lubricant moving out friction and correction of sample flow pattern has been used by last experimental studies (Zhou et al. 2017). In this respect: (1) Imposed thermomechanical cycles to samples consist of austenite treatment lasted 7.5 min in temperature of 1423 k (2) cooling up to deformation temperature in 1373, 1273, 1173 k and also imposing strain value (= 0.9) which their strain rates was respectively = 0.01, 0. 1, 0.5, 1 s-1. Finally, all specimens were cooled from deformation temperature at constant and time (5 min) to environmental temperature. Optimum results of thermomechanical test consist of strain – stress curves. Stress – strain curves indicate flow behaviors of material in various temperatures and strain rate so, effect of strain rate and temperature in all thermomechanical cycles have been evaluated.

ARTIFICIAL NEURAL NETWORK ARCHITECTURE

A feed-forward multilayer perceptron (MLP) with back-propagation algorithm was designed and developed with Matlab software. The given input parameters are temperature, strain rate and strain of the 40NICRMO8-4 alloy. Likewise, flow stresses of the desired alloy were expected to be predicted by the modeled network as the outputs of the system. Figure 2. illustrates a simplified graph of the inputs and the output.

By following the standard procedure of modeling an ANNs, a training set along with an independent validation set in order to evaluate the generalization property of the trained network was utilized. It is crucial to give normalized inputs ranged between 0 and 1 or -1 and 1 to an ANN.

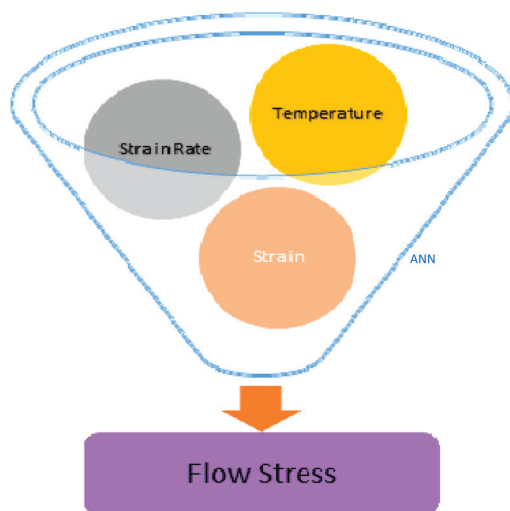


FIGURE 2. Simplified schematic of inputs and outputs of the ANN model of this study

Main reason to this process is to bring all various inputs from different ranges into one unique range to help the neural network treat them fairly and inputs with large or small values affect the network training and consequently variables with large values bias the training process and the results will not be reliable. In this study, equation 1 was used to normalize all the data between 0.1 and 0.9. According to this reason, all values were normalized by applying equation 1 on them. Therefore, all the values were set to be between 0.1 and 0.9.

$$X_n = \frac{0.1 + 0.8(X - X_{\min})}{(X_{\max} - X_{\min})} \quad (1)$$

This equation guarantees that the normalized value (X_n) is placed somewhere in between X_{\min} and X_{\max} . Reverse step is taken after reaching the desired network model leading to original values of outputs. To this end, equation 2 is employed to obtain original values from normalized ones.

$$X = \frac{(X_n - 0.1)(X_{\max} - X_{\min})}{0.8} + X_{\min} \quad (2)$$

The objective of standardization is to eliminate differences of units by moving to a dimensionless domain leading to canceling out the random effect of similarity between the properties. Furthermore, there exist only one neuron in the output layer providing us the desired property which is flow stress of the desired alloy (Lin et al. 2009). Sigmoid function was chosen as transfer function for hidden layers. It has been proved that every ANNs employing sigmoid function in their hidden layers while using linear function for the output layer can track every function with finite discrete points if hidden layers contain enough nodes (Eiben and Smith, 2003). Equation 3 represents the sigmoid transfer function:

$$f(s) = \frac{1}{1 + \exp(-s)} \quad (3)$$

Figure 3 illustrates a sigmoid function. Omit this part, this function softly tends to a constant value as S increases and becomes almost zero at negative infinity. Nevertheless, there exist sharp fluctuations in terms of values around the middle of the graph. So, sigmoid function is considered as a soft rounded threshold when it comes to comparison with other transfer functions.

As it mentioned above, transfer function for output layer was chosen to be pure line function for its unique properties. In prediction applications it is not desirable to limit the output values. Hence, sigmoid function is best to be avoided for being used in output layer. But, by employing linear transfer function for output neurons, network can get any value (Zakeri et al. 2007). Equation 4 shows the dominant relationship between input and output of a linear function. Equation 4 shows the relationship between input and output of a linear function while figure 4 represents its pertaining plot.

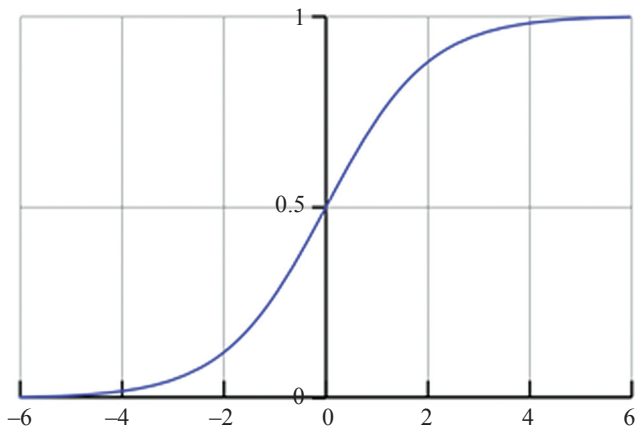
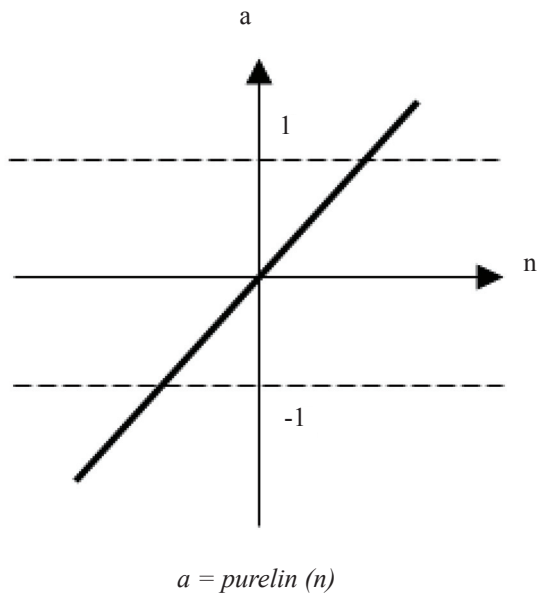


FIGURE 3. Sigmoid function



$$a = \text{purelin}(n)$$

FIGURE 4. Pure-line function employed in the output layer

$$Y_{\text{linear}} = X \tag{4}$$

Two models for the ANNs of this study were employed consisting of 1 and 2 hidden layers which Figure 5 shows the schematic view of the one with two hidden layers in MATLAB software.

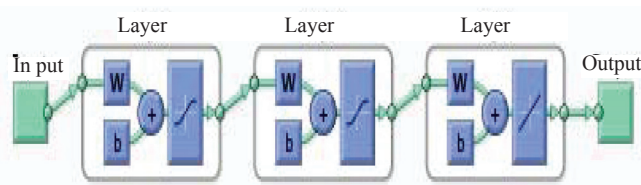


FIGURE 5. Two-layer tan sig/pure-line network schematic view in MATLAB

To evaluate the network performance, mean square error (MSE) parameter was selected as the key identifier of the best architecture (Yang et al. 2012). MSE is widely used in studies

to evaluate performance of a system or method. The formula for calculating the MSE of our designed networks has been given in equation 5.

$$MSE = \frac{1}{p} \sum_{j=1}^p [y_j^d - y_j^o]^2 \tag{5}$$

where y^d is the target value, y^o is the obtained value from ANNs, and p is the pattern presented. There were 214 samples available in our dataset. Following the standard procedure of training an ANN, this dataset was divided into 3 groups as train, test and validation subsets at first. 60 percent of the dataset which contains 128 data were chosen to be used as train set and 20 percent (43 data) for testing the trained network. The remained 20 percent were also used for validation of the network. In addition, a momentum rate of 0.6 and learning rate of 0.3 were set for the models.

Data from training set are selected randomly for each epoch in order to avoid the network to be biased based on specific data order. Levenberg-Marquardt was also chosen as training algorithm due to its quick convergence and small MSE. One of the most common errors may happen during modeling an ANNs is overfitting or underfitting. Moreover, there is no specific and clear routine to follow in order to reach the best design. Hence, it is necessary to test different architectures in terms of the number of hidden layers and the neurons in each of them to get the best result.

As mentioned earlier, ANNs with 1 and 2 hidden layers with the mentioned configuration were employed. The numbers of neurons in each layer were also altered from 3 to 15 in order to check the effect of hidden layers and neurons on network performance. In total, there were 182 networks to compare their results with each other. It goes without saying that in each run, the best result may be different from the previous run as the weights of networks initialized with random values. There is also another step following this step which is to put the chosen network under further training for about 20 times to achieve even more accurate results as well as optimizing other parameters. Next section will discuss the outcomes of the afore-mentioned procedures.

RESULTS AND DISCUSSION

THERMOMECHANICAL PROCESS

Experimental results of Thermomechanical process of 40NICRMO8-4 alloy steel in various strain rate and temperature based on true stress- strain curve has been determined as in Table 2.

EFFECT OF STRAIN RATE

As figure 6 shows, the increase in strain rate will result in the increase in stress. In one specific strain, when sample strain rate increases, the sample will reach into higher level of energy.

As a result, dislocation speed will increase and thereafter, dislocations will hit to the blockages much sooner and finally

TABLE 2. Experimental results after normalization

$\dot{\epsilon}^o (s^{-1})$	T(K)	Softening Mechanism	$F_{max} (N)$	$\sigma_{Max} (N/mm^2)$
0.01	1373	Dynamic recrystallization (steady state)	1448	35.7
	1273	Dynamic recrystallization (steady state)	2281	54.6
	1173	Dynamic recrystallization (non-steady state)	4361	92.5
0.1	1373	Dynamic recrystallization (steady state)	2159	53.1
	1273	Dynamic recrystallization (non-steady state)	4611	107
	1173	Dynamic Recovery	8217	167.9
0.5	1373	Dynamic recrystallization (non-steady state)	4201	98.4
	1273	Dynamic Recovery	6618	136.7
	1173	Dynamic Recovery	9661	195.4
1	1373	Dynamic recrystallization (non-steady state)	4764	106.1
	1273	Dynamic Recovery	7314	148.9
	1173	Dynamic Recovery	9801	199.8

will stop. Dislocation density will be increased more because of this stoppage. Direct influence of this is to increase flow stress (Beladi et al. 2017). And also increasing in strain rate when temperature is constant, recrystallization will happen in more strains at times shorter. That is to say, it will take place with delay.

Raising of strain rate sensitivity in high temperature is related to the raising of process rates activated by heat. Process such as dislocation climb and grain slip are the best ones to mention. Figure 7 also shows the relationship between strain rate sensitivity and temperature. Rising in strain rate sensitivity value can be due to DRX in high temperature where they have high strain rate sensitivity value compared to low temperature (Lorenz et al. 2003; Salehi et al. 2006).

TEMPERATURE EFFECT

As shown in Figure 7, temperature clearly influence on flow stress. When temperature rises, dislocation movement can easily happen. This results in decreasing dislocation density. Therefore, flow stress for every strain value is less than low temperature and material resistance against deformation will also decrease (Lee et al. 2006).

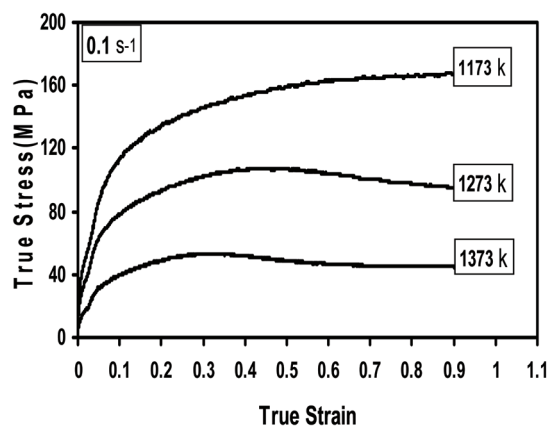


FIGURE 7. The effect of temperature on the strain-stress graph in $0.1 s^{-1}$

As can be seen in Figure 7, when strain value is constant, recovery process as temperature raises will change into dynamic recrystallization. That is because, as temperature rises, it can cause to increase in nucleation and growth speed. In fact, if the temperature increases, activation of atoms will grow. So, subgrain boundary and anile twins can act as main centers of recrystallization nucleation formation and can quickly be formed to accelerate dynamic recrystallization (Mohammed et al. 2014).

PREDICTION OF TEST DATASETS EMPLOYING MODELLED ANN

This section in turn, discusses the achieved results from the modeled network. As mentioned in previous section, defined ANNs with 1 and 2 hidden layers set based on the chosen configurations, were implemented and run to give us the predicted values. Figure 8 illustrates obtained MSE values for a simple comparison while Table 3 depicts the best obtained MSE values of the modelled ANNs.

As can be seen, most of the networks could provide us a reasonable accuracy in predicting strain values but it is also obvious from the stats that employing 2 hidden layers leads to better results. Likewise, it is usually expected to achieve better results by increasing the number of nodes in hidden layers, but by referring to the results, it can be concluded that this statement is not necessarily true for all conditions. When there exists only one hidden layer, by adding more neurons to the layer, better results are expected, but, speaking of ANNs with more hidden layers, it cannot be concluded like that.

However, it is of great importance to know that depending on the objectives of the study, minimum MSE may not be the only key factor in choosing the best model for ANNs but other factors such as the learning and momentum rates play crucial roles especially on quickening the convergence speed (Rajabi et al. 2012; Sabokpa et al. 2012).

By checking the results, it was noticed that a back propagation neural network (BPNN) with structure of 3-12-7-1 lead to the best results against the other networks. This network gave an R value of 0.99871 which is indeed a perfect prediction. R, or so-called correlation coefficient, is to measure the correlation between predicted results and real

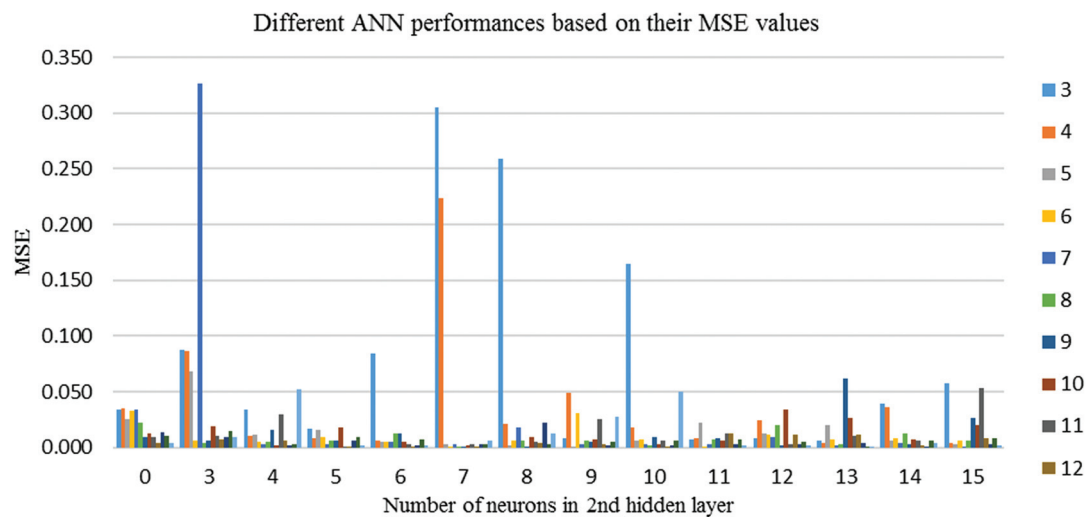


FIGURE 8. Obtained MSE values of the proposed ANN with different number of hidden layers as well as different neurons per hidden layers

data and it is a way to figure out how accurate could your network predict the results. Figures 9, 10 and 11 demonstrate the obtained results of the mentioned network.

As the results revealed, small networks are incapable of modeling the process perfectly due to their limited degree of freedom to learn the process. Similarly, large networks introduce unnecessary complexity to the model and lead to

overfitting phenomenon. Therefore, a network is required which is trained properly to relate the inputs to outputs in a proper manner to fulfill the goals of the system.

CONCLUSION

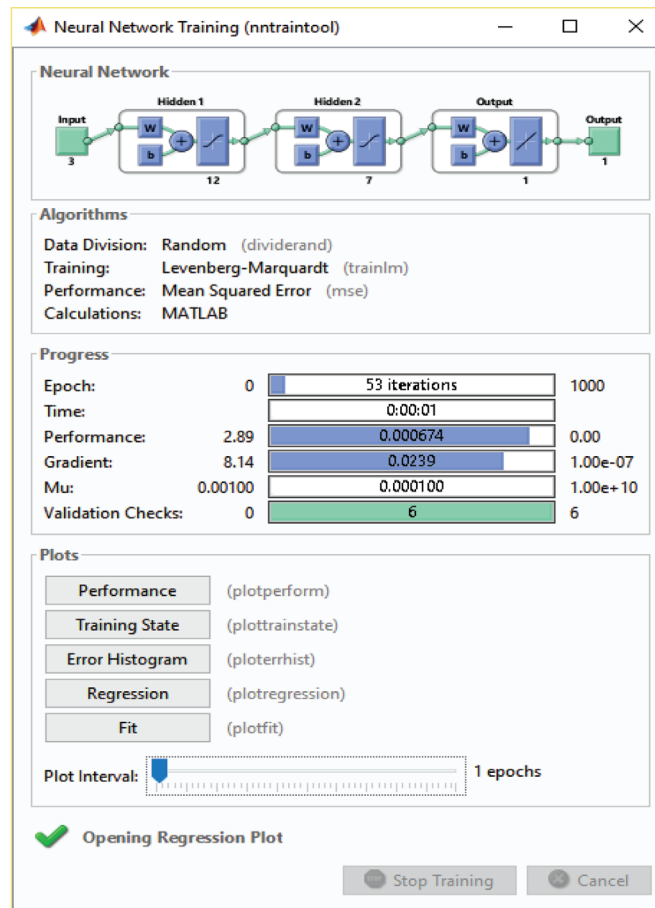
Flow stress for every strain value at high temperatures is less than at low temperatures and material resistance against deformation will also decrease. Any increase in temperature while keeping strain value constant leads to transformation of recovery process into dynamic recrystallization. And also increasing in strain rate when temperature is constant, recrystallization will happen in more strains at times shorter. Additionally, results provided by the study revealed that a feed-forward MLP is capable of modeling the thermomechanical process of 40NICRMO8-4 alloy and can save money and time. A BPNN network with structure of 3-12-7-1 showed an excellent convergence giving a R_{testing} value of 0.99871 in predicting flow stress values which is an impressive result of its own kind. Either small or extremely large networks are not good choice for our goal as they both have some shortcomings such as insufficient degree of freedom or overfitting issue. Moreover, the complexity of the thermomechanical process induced by the interaction of numerous parameters simultaneously (e.g., material composition, strain rate and temperature) causes difficulty in obtaining accurate experimental results. Nevertheless, the study results showed that ANNs are capable of figuring out the relation between mechanical properties of 40NICRMO8-4 alloy in order to forecast the output results with high accuracy and reliability.

ACKNOWLEDGEMENT

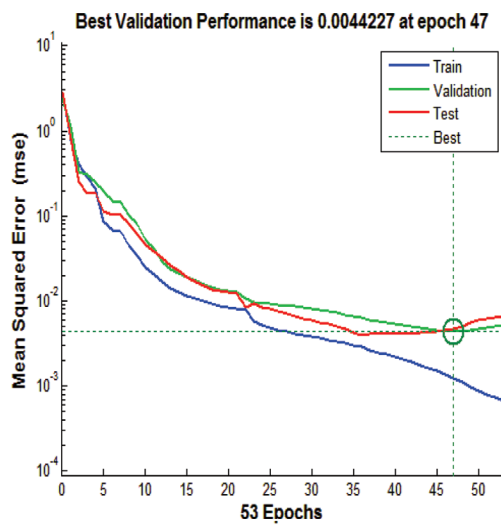
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TABLE 3. Predicted MSE values of the system employing different number of layers and neurons per layer

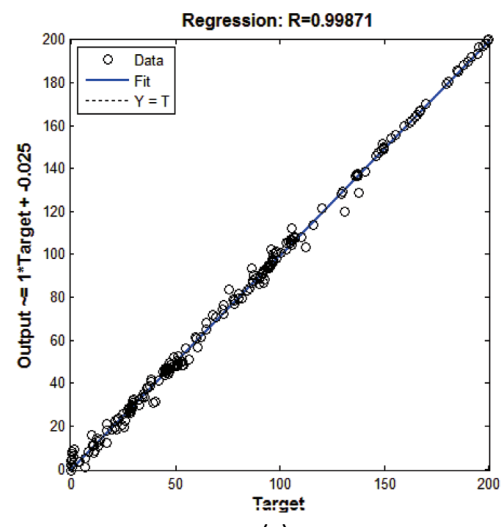
Number of hidden layers	ANNs structure	MSE value
1	3-3-1	0.033818
	3-4-1	0.034939
	3-5-1	0.025536
	3-6-1	0.033411
	3-7-1	0.033754
	3-8-1	0.022525
	3-9-1	0.009592
	3-10-1	0.012288
	3-11-1	0.009864
	3-12-1	0.004575
	3-13-1	0.013735
	3-14-1	0.010946
	3-15-1	0.003799
	2	3-3-8-1
3-4-10-1		0.001727
3-5-12-1		0.000507
3-6-12-1		0.000644
3-7-12-1		0.000052
3-8-9-1		0.000681
3-9-5-1		0.000366
3-10-12-1		0.001133
3-11-6-1		0.000346
3-12-9-1		0.002021
3-13-15-1		0.000718
3-14-13-1		0.001250
3-15-7-1	0.000517	



(a)



(b)



(c)

FIGURE 9. (a) ntraintool window of the best ANN, (b) Performance chart of the best ANN
(c) Regression plot of the best ANN

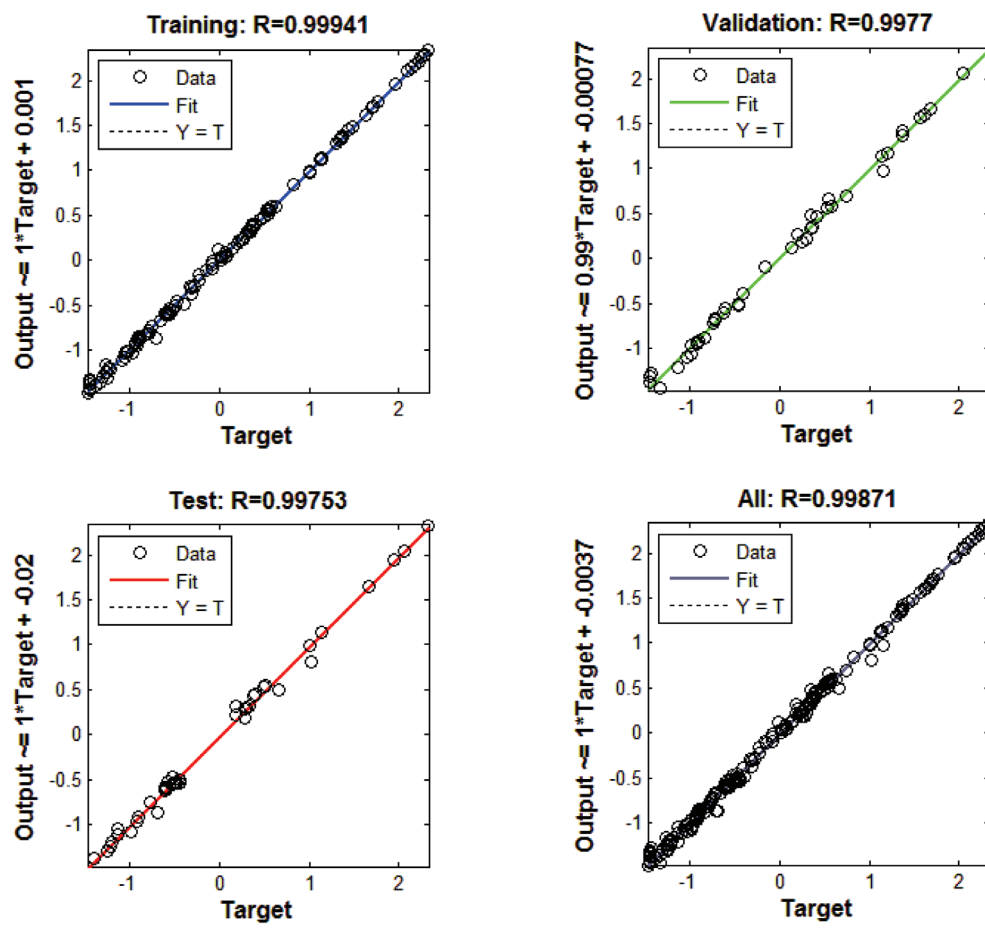


FIGURE 10. R values of the chosen ANN with best performance

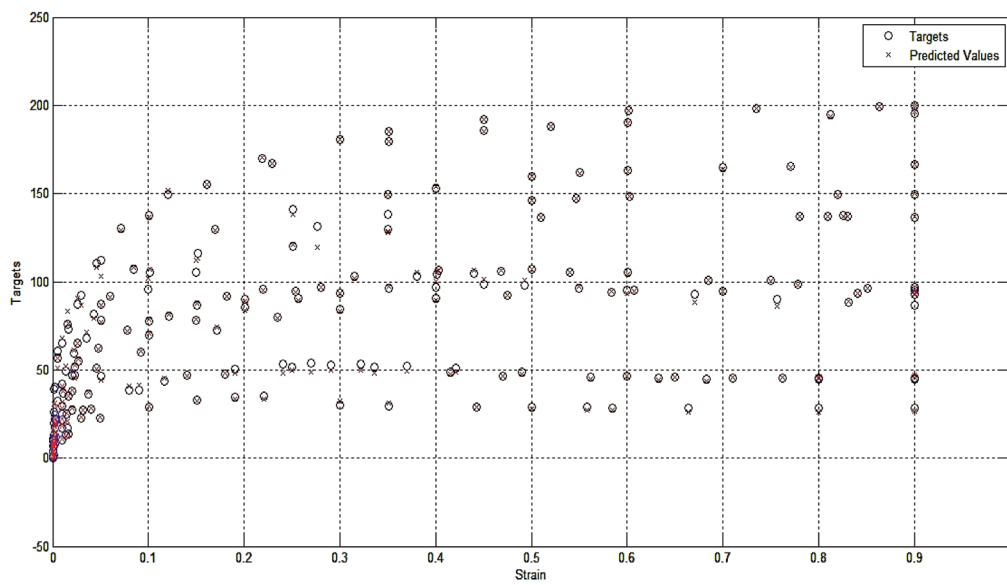


FIGURE 11. Predicted values of the chosen ANN vs. targets

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