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Modeling constitutive behavior of a 15Cr-15Ni-2.2Mo-Ti modified austenitic stainless steel under hot compression using artificial neural network

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ABSTRACT

In this paper, an artificial neural network (ANN) model has been suggested to predict the constitutive flow behavior of a 15Cr-15Ni-2.2Mo-Ti modified austenitic stainless steel under hot deformation. Hot compression tests in the temperature range 850°C-1250°C and strain rate range 10^{-3}-10^{2} s^{-1} were carried out. These tests provided the required data for training the neural network and for subsequent testing. The inputs of the neural network are strain, log strain rate and temperature while flow stress is obtained as output. A three layer feed-forward network with ten neurons in a single hidden layer and back-propagation learning algorithm has been employed. A very good correlation between experimental and predicted result has been obtained. The effect of temperature and strain rate on flow behavior has been simulated employing the ANN model. The results have been found to be consistent with the metallurgical trend. Finally, a monte carlo analiysis has been carried out to find out the noise sensitivity of the developed model.

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1. Introduction

Austenitic stainless steels, primarily AISI 316 and its modifications, have been selected world-wide as prime candidate materials for fuel cladding and sub-assembly wrapper tubes of fast breeder reactors. For the 500 MWe fast breeder reactor project (PFBR) in India, a 15Cr-15Ni-2.2Mo-0.3Ti austenitic stainless steel has been developed indigenously. This conforms to ASTM A771 UNS 38660 and is commonly referred to as alloy D9. This is a candidate material for in-core applications as fuel cladding tube and hexagonal subassembly wrapper. Alloy D9 has to be processed through various thermo-mechanical treatment before it is fabricated into final component. However, the high temperature deformation behaviour of alloy D9 is associated with various complicated metallurgical phenomena like work hardening (WH), dynamic recovery (DRV), dynamic recrystallization (DRX), flow instabilities etc. and thereby complex in nature. Therefore, understanding of the constitutive flow behavior is required in order to avoid flow instabilities in the deforming materials and to get a defect free end product.

In past, various internal state variables phenomenological models [1-3] or empirical/semi-empirical equations [4-6] have been constructed to predict the constitutive flow behavior of materials during hot working. Although these approach attempt to represent the non-linear relations between flow stress (σ), strain rate ($\dot{\varepsilon}$), strain (ε) and temperature (T), they are usually restricted to some limited processing domain where a specific deformation mechanism operates and break down across deformation mechanism domains. Therefore, separate equations and/or various equation parameters are needed to represent the complete hot deformation behavior.

Artificial neural network (ANN), in this respect, provides an efficient alternative. ANN utilities a statistical approch to modeling and is one of the most powerful modern modeling techniques. The basic advantage of ANN is that it does not need any mathematical model; an ANN learns from examples and recognizes patterns in a series of input and output values without any prior assumptions about their nature and interrelations. Since ANN does not explicitly embed the physical knowledge of the deformation mechanism, it has the ability to predict the flow stress value across the deformation domains. Therefore, a single ANN has the inherent capabilities to describe the complete hot deformation behavior. In this study, therefore, an ANN model is suggested to predict the constitutive flow behavior of alloy D9 during hot deformation.

2. Experimental

The chemical composition of alloy D9 used in this investigation is given in Table I. The thermomechanical treatments employed for this material are the same as reported elsewhere [7]. Compression specimens of 15 mm height and 10 mm diameter were machined for testing. Isothermal hot compression tests were conducted using a computer controlled servohydraulic testing machine (DARTEC, Stourbridge, UK) with a maximum load capacity of 100 kN. The testing temperatures ranged from 850-1250^{o}C at an interval of 50^{o}C and at constant true strain rates 0.001, 0.01, 0.1, 1, 10 and 100 s^{-1}. The specimens were deformed to half the height in each case to impose a true strain of 0.7. The load-stroke data obtained in compression were processed to obtain true stress-true plastic strain using standard equations. Table II gives the statistical analysis of the flow stress data as a function of strain, strain rate and temperature.

Table I: Chemical compositions (in wt. %) of alloy D9

C	Mn	Si	S	P	Cr	Ni	Mo	Ti	B	N
0.052	1.509	0.505	0.002	0.011	15.05	15.07	2.25	0.3	0.001	0.006

Table I1: Statistical analysis of input and output data

Variables	Maximum	Minimum	Stand. Dev.	Average
Strain (%)	0.5	0.1	0.142	0.3
Strain rate (s^{-1})	100	0.001	40.10	18.52
Temperature (^{o}C)	1250	850	129.34	1050
Flow stress (MPa)	446.1	17.6	107.01	178.56

3. Model overview

ANN is a highly simplified model of the structure of a biological network. The fundamental unit or building block of ANN is the processing element, also called an artificial neuron or simply a neuron. Some neurons interact with the real world to receive input, and some provide the real world with the output. Rest of the neurons remains hidden. Neurons are connected to each other by synapses; associated with each synapse is a weight factor. More details regarding ANN modeling can be found elsewhere [8].

In this study, a multilayer perceptron (MLP) based feed-forward ANN has been used since multilayer network has greater representational power for dealing with highly non-linear, strongly coupled, multivariable system [9]. A general scheme of the present ANN model is given in Fig.1. The inputs of the model are strain (ε), log strain rate ($\log\dot{\varepsilon}$) and temperature (T). The output of the model is flow stress (σ). Instead of $\dot{\varepsilon}$, $\log\dot{\varepsilon}$ has been chosen since σ usually varies with $\log\dot{\varepsilon}$ on a physical basis [10].

A total of 270 input/output data points have been employed in the present study. All datasets (ε, $\log\dot{\varepsilon}$, T and σ) were scaled between 0 to 1 in order to ensure that each variables lie in the same range during training and testing. Theses datasets were then divided into two parts. 25% of the datasets were randomly removed and remaining 75% were used for training. The removed 25% datasets were subsequently used for testing. After repeated trials, it was found that a network with one hidden layer consisting of 10 hidden neurons produces best performances and thereby considered as the optimal configuration for the present problem. This observation reaffirms the universal approximation theorem that a single layer of non-linear hidden units is sufficient to approximate any continuous function. A logistic sigmoid function expressed as $Output = (1 + e^{-input})^{-1}$ was employed as the activation function; the learning is based on gradient descent algorithm and hence requires the activation function to be differentiable.

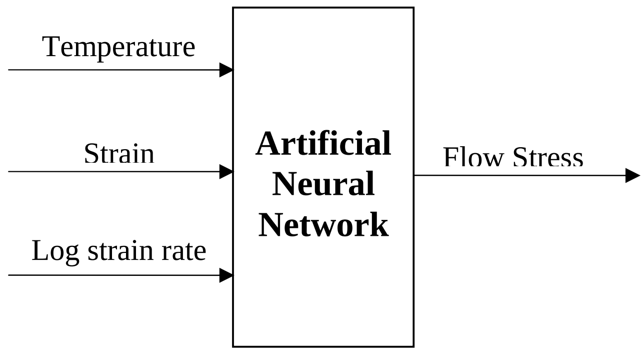

Figure 1: Schematic of the ANN for flow stress prediction in alloy D9

4. Learning algorithm

Back Propagation (BP) learning algorithm has been used to train the model. The basic idea of BP learning algorithm consists of repeated application of chain rule to compute the influence of individual weight in the network with respect to error energy E^n :

$$\frac{\partial E^n}{\partial w_{ji}^n} = \frac{\partial E^n}{\partial e_j^n} \frac{\partial e_j^n}{\partial y_j^n} \frac{\partial y_j^n}{\partial v_j^n} \frac{\partial v_j^n}{\partial w_{ji}^n} \qquad (1)$$

In the above, w_{ji}^n is the weight from neuron i to neuron j at iteration n; e_j^n refers to the error signal at the output of neuron j at iteration n; and v_j^n is the weighted sum of all synaptic inputs of neuron j at iteration n. Once the partial derivative for each weight is known, error energy is minimized through a gradient descent:

$$\Delta w_{ji}^n = -\alpha \frac{\partial E^n}{\partial w_{ji}^n} \qquad (2)$$

where α is learning rate.

The convergence criterion for the network is determined by the average root-mean-square (RMS) error between the desired and predicted output values,

$$E_{RMS} = \frac{1}{N} \sum_{i=1}^{N} \sqrt{\frac{1}{p} \sum_{j=1}^{p} (d_{ji} - y_{ji})^2} \qquad (3)$$

where E_{RMS} is the average root-mean-square, N is the number of training or testing data and p is the number of variable in the output. In all the calculations reported in this paper, a convergence criterion of 1% RMS error has been set. But invariably it is found that the network stabilizes before this criterion is met.

5. Results and Discussion

The sailent features of the model is shown in Table III. The predictability of the network is shown in the form of linear regression between the experimental data and corresponding predicted result for both the training and test datasets (Fig.2 and Fig.3 respectively). The results show that a very good correlation between experimental and predicted data has been obtained. Predicted result could efficiently track the experimented data over the full range of datasets.

Table III: Sailent features of the ANN model to predict the constitutive behavior of alloy D9

Algorithm	Learning rate	Weight initial^{n}	Iterations	RMS Training Error (%)	R (Training)
BP	0.1	± 0.1	10,000	6.01	0.997

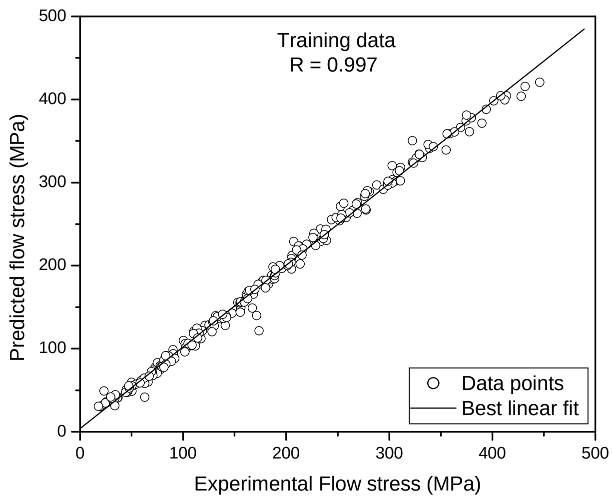

Figure 2: Correlation between experimental and predicted training data for flow stress prediction in alloy D9

The performance of the model is further demonstrated by statistical analysis of the error of neural network predictions for both the training and testing data. Neural network predictions are compared with the corresponding experimental data and subsequently the relative errors are calculated as below:

$$\text{Relative Error} = \left(\frac{E-P}{E}\right) \times 100\%, \qquad (4)$$

where E is the experimental output value and P is the predicted value obtained from the neural network model.

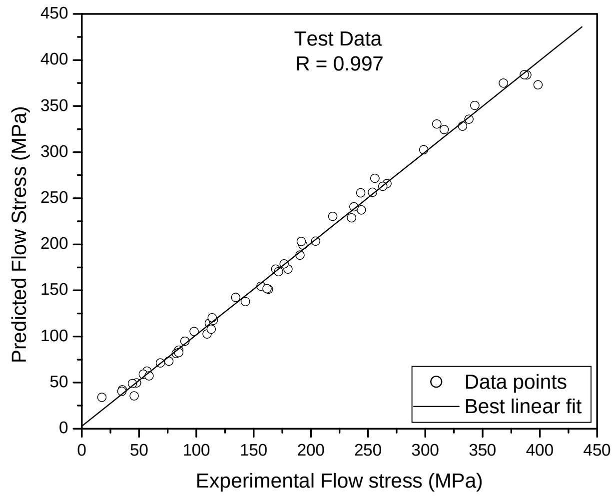

Figure 3: Correlation between experimental and predicted test data for flow stress prediction in alloy D9

It has been observed that the error shows a Gaussian distribution with zero mean. For more than 90% training and test data set, the error of prediction is found to be within $\pm 10\%$. This signifies that main source of prediction error is the noise in the experimental data which has been fed to train and test the ANN model and hence can not be wholly attributed to the predictability of the neural network model. The small noise in flow stress measurements can readily arises due to unavoidable variations in temperature, strain rate and interfacial friction resistance [11].

It should be kept in mind that a robust ANN model can be efficiently developed by proper selection of input and output variables, adequete input informations and comprehensive database. However, the amounts of database or information required depend on the complexity of the problem being modeled and thereby not deterministic. For example, in the present problem, a set of 270 input/output data points have been found to yield a very good correlation in a wide ragne of deforming conditions. The same problem, also, can be modeled with lesser number of data points. However, as ANN is a non-linear statistical modeling technique, the cofidence limit and therby prediction accuracy will go down with the lesser number of data density.

It is a matter of debate among the researcher whether ANN model should be used for extrapolation or not. Since ANN purely learns from examples, the predictibility of model would definitely be high with in the training domain. However, in our recent study, we have shown that ANN can also efficiently extrapolate as long as underlying mechanisms do not change for the extrapolated data [12]. On the other hand, prediction was found to be detoriated when there is changes in the underlying mechanism in the extrapolated regime. Therefore, it is concluded that extrapolation of ANN model should be carried out with great caution.

5.1 Effect of temperature and strain rate

The effect of temperature and strain rate on flow behavior of alloy D9 has been simulated employing the developed ANN model. The result has been shown in Fig.4 and Fig.5 respectively. As can be seen from the figures, simulated curve can track well the experimented data. With increase of temperature, flow stress decreases in both the highest and lowest strain rate (Fig.4). Similar kind of trends have been obtained in other strain rates and therefore not iterated. The predicted dependence on temperature is in accordance with the relation between flow stress and temperature. As the temperature increaes, the available thermal activation energy will be more which eventually leads to higher extent of dynamic softening. This dynamic softening may arise either from DRV or DRX. On the other hand, with increase of strain rate flow stress increases because of higher extent of work hardening (Fig.5). The simulated results are therefore consistent with what is expected from fundamental theory of hot deformation. These results also suggested that our model could efficiently predict the flow behavior accross the deformation mechanism domain (WH, DRX, DRV or flow localization) and therefore capable to predict the complete hot deformation behavior of alloy D9.

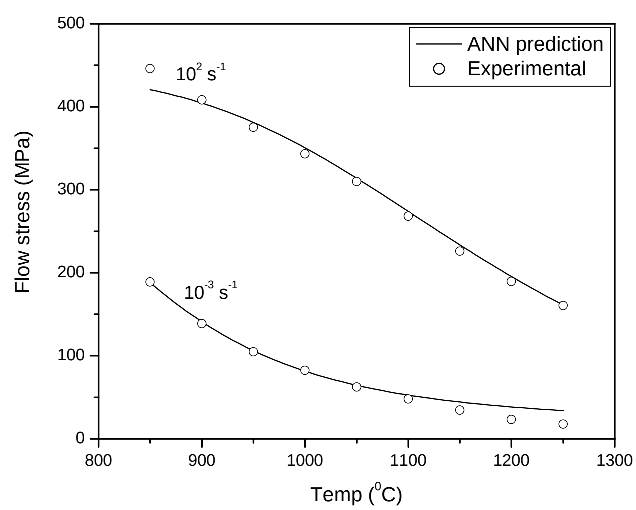

Figure 4: Effect of temperature on constitutive flow behavior of alloy D9 at 0.5 strain

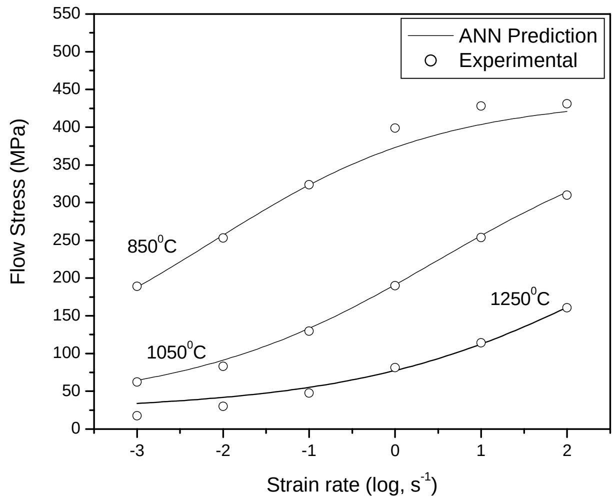

Figure 5: Effect of strain rate on constitutive flow behavior of alloy D9 at 0.5 strain

5.2 Sensitivity analysis

To investigate how sensitive ANN is to fluctuations in the input data, the following Monte Carlo analysis was carried out. We select nominal values of the three input parameters: $\hat{T} = 925°C$; $\hat{\varepsilon} = 0.3$; $\hat{\dot{\varepsilon}} = 100\,s^{-1}$. We assume T, ε and $\dot{\varepsilon}$ to be Gaussian random variables with mean equal to $\hat{T}$, $\hat{\varepsilon}$, $\hat{\dot{\varepsilon}}$ and 5% relative standard deviation. T, ε and $\dot{\varepsilon}$ is sampled independently and randomly from their respective distribution and fed as inputs to the ANN which returns flow stress (σ) as output. This exercise was carried out 1000 times. The mean and standard deviation of σ is found to be 369.29 MPa and 5.58% respectively. σ Corresponds to nominal value is 371.47 MPa which is well within the fluctuations. From the analysis, therefore, it could be concluded that the fluctuations in σ (5.58%) is approximately the same as fluctuation in the input parameters (5%).

6. Conclusions

An artificial neural network model has been constructed for the prediction of flow stress of 15Cr-15Ni-2.2Mo-Ti modified austenitic stainless steel (alloy D9) using experimental data from hot compression testing. Various network configurations were tried and an ANN model with one hidden layer and ten hidden neurons was found to be optimal configuration when strain, strain rate and temperature are input parameter. It has been shown that the ANN model is capable to predict the complete flow behavior of alloy D9 with sufficient accuracy. This can be considered as major potential of the developed ANN model as compared to phenomenologcal or traditional regression analysis whcih can be apllied to a limited processing domain.

The sensitivity of ANN on the fluctuations in input data has also been investigated. It has been found that fluctuation in the output parameter is approximately same as that of inputs.

The outcomes of this model give us enough confidence to employ ANN in predicting flow stress during high temperature deformation. This implies that experimental studies can be reduced significantly which would save considerably money and man power required for extensive experimentation.

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