Prediction of Fracture Energy of IN738LC Superalloy using Neural Networks

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Abstract: IN738LC is a cast polycrystalline nickel based super alloy, primarily used for first stage gas turbine blades which operate under severe loading conditions and temperatures. The development of relationship among operating temperature, microstructure and mechanical properties of the material is very important in order to understand its failure mechanisms and fracture behavior. For this purpose, this paper presents a three layered feed forward back propagation neural network model capable of predicting the fracture energy of IN738LC. Temperature, strain rate, gamma prime precipitate size, yield strength, ultimate tensile strength and percentage elongation to failure taken from literature are used to train, validate and test the model. Results obtained from the neural network model describe experimental values accurately for given operating conditions. Therefore, it can be used to correlate microstructural parameters to strength and toughness properties under real operating conditions.

1. Introduction

Gas turbines and aerospace engines operate at high temperatures and under severe thermal and mechanical loading conditions which can result in failure of the material. Temperature, mechanical properties (yield strength, tensile strength etc) and microstructure of materials used at high temperatures are fundamental parameters in the design and assessment of aerospace components. Such components, particularly gas turbine blades, are usually made of the cast polycrystalline nickel base superalloy IN738LC (Inconel 738 Low Carbon). The intermetallic gamma prime (γ') precipitates, ($Ni_3Al/Ti/Nb$), are the main hardening particles within the gamma (γ) matrix. The size, morphology and thermal stability of the γ' precipitates are determining factors for all high temperature properties of the material [1]. The desired γ' precipitate structures such as fine (F), medium (M), coarse (C) and duplex (D) can be obtained by different heat treatments. For instance, simple solution heat treatment at 1200^{o}C for 4 hours followed by water quenching (WQ) produces fine precipitates. Reheating and maintaining solution heat treated samples at 900^{o}C and 1120^{o}C for another 24 hours result in medium and coarse size precipitates, respectively. Reheating the coarse precipitate material for an additional 6 hours at 1140^{o}C results in a duplex microstructure in which the coarse-sized precipitates are partially dissolved into the matrix creating fine secondary precipitates [2]. In the context of this paper, these microstructures obtained at different conditions of temperature can be correlated to strain rates, mechanical properties and fracture energy (fracture toughness), or the energy to break the material. At low strain rates, fine and duplex precipitates show higher yield strength, but lower fracture energy as compared to medium and coarse precipitates due to easy occurrence of a cleavage type fracture on the {100} planes at low temperature and on the {111} slip planes at high temperature. At high strain rates, there is an increase in fracture energy at 650^{o}C. Above this temperature, the fracture energy decreases drastically. The degree of toughness drop or increase greatly depends on the type of microstructure. Coarse precipitates show the highest fracture energy at 650^{o}C probably due to either the highest ductility associated or of the specific vacuum heat treatment used for the production of this microstructure that prevents oxidation during heat treatment. Medium and coarse precipitate microstructures generally show more dimple-ductile type fracture at all temperatures which can well be correlated to higher fracture toughness values. In contrast, fine and duplex precipitate structures show lower toughness values and cleavage type fracture [3].

Various quantitative models can be useful in determining the fracture energy, assisting in the prediction of fracture behavior of nickel based super alloys and reducing the need for experimental work. A neural network is one of the most promising methods in achieving this goal [4].

An artificial neural networks is used in the current paper. It is a computer intensive blind modeling technique [4]. It is a fast, flexible, efficient and accurate tool to predict and model highly nonlinear multidimensional relationships. Due to flexible modeling and learning capabilities of neural networks, it is possible to solve complex problems without any mathematical relationships between inputs and outputs. Neural networks is presently successfully used in a wide range of applications such as medical, military, space, and much more [5].

2. Neural Networks

An artificial neural networks works in accordance with the human brain. It has nonlinear basic processing units called neurons. These neurons are connected by weights and biases and are arranged into layers [6]. Basically, the neural network architecture consists of multiple layers of neurons, i.e. an input layer, an output layer and one or more hidden layers between them. The number of neurons in the input layer is determined from the number of input variables. The neurons in the hidden layer are determined by trial and error with various weights and biases, whereas the number of targets (or the output to be determined) is considered to be the number of neurons in the output layer. Generally, underfitting occurs if the hidden neurons are too few and too many neurons causes overfitting because the network is very sensitive to the number of neurons in the hidden layers and can cause strong oscillations [7].

The most commonly used neural network architecture is multilayered feed forward back propagation because it requires smaller training sets, is easy to implement and execution time is low. The back propagation training set has input vectors and corresponding target vectors [7]. It has two phases during training, mainly, the forward phase and the backward phase. In the forward phase, the input vectors of the training set are moved forward through the network layers. The output is computed by the network for each input in the training set. The error or difference between the target (actual expected output) and computed output is determined. In the backward phase, the error is subsequently back propagated from the output layer to the hidden layers and weights and biases are updated. This process is repeated many times until the error is minimal for the network for the defined goal, epoch or other parameters [5].

During training, the error in a specific training set can be small, but the error can still be very large when new input data are fed to the network. This is called overfitting and can be avoided by dividing the total data set into three subsets: a training subset (50% of the total data set), a validation subset (25% of the total data set), and a test subset (25% of the total data set). The training subsets are used to compute the error and update the network weights and biases, i.e. to train the network. Initially, the error in both validation and training subset decreases, but as the error in the validation subset begins to rise after a specified number of iterations in cases where the network overfits the data and the training is stopped at that point. In this way, the validation data set plays a major role to avoid overfitting. The test subset is used to assess the generalization error and to compare the results [7].

Feed forward Levenberg-Marquadt back propagation algorithm, a numerical optimization technique, is used in the present work to iteratively update the weights and biases to minimize the error i.e. mean squared error (MSE) which is a performance function of this algorithm. Levenberg-Marquadt algorithm is a variation of the Newton's method by introducing the new scalar parameter μ (mu). The training parameters for this training algorithm are epochs, show, goal, mu, mu_dec (μ decreased), mu_inc (μ increased), mu_max (μ maximum), mem_reduc (memory reduction) etc. The training status is displayed in every show. The most important parameter is mu which is decreased or increased to reduce the performance function during training of the network. Training stops when some predefined conditions are met i.e. mu becomes larger than mu_max, the number of iterations exceed epochs, the performance function reaches the goal, etc. Levenberg-Marquadt back propagation algorithm is the fastest training algorithm available. But, it also requires a lot of memory when the training set is large. Therefore, the parameter mem_reduc is used for the reduction of memory requirement [7].

3. Neural Network Modeling

In this paper, an artificial neural network (ANN) model based on experimental data is developed to predict average static fracture energy of IN738LC. The experimental data set in Table 1 is used as inputs and target for training. Temperature, stain rate, tensile properties (yield strength, ultimate tensile strength, and percentage elongation to failure) and microstructure (including both primary and secondary precipitate size) of four different γ' precipitate structures are the inputs. The average static fracture energy obtained from tensile load-displacement test for different strain rate and temperatures is taken as the target [3].

Table 1: Inputs and Target values for IN738LC [3]

INPUTS						TARGET
Microstructure	Temperature (^{0}C)	Strain Rate S^{-1}	Yield Strength σ_Y (MPa)	Tensile Strength σ_T (MPa)	Elongation (%)	Fracture Energy (Joule)
Fine (F)	20-850	$5\ 10^{-5}$	552-859	553-965	4.7-11.2	6.0-14
70nm	20-850	10^{-3}	684-852	685-916	4.7-16.0	9.0-58
Duplex (D)	20-850	$5\ 10^{-5}$	634-834	654-913	5.1-12.1	9.0-38
(50 and 450 nm)	20-850	10^{-3}	762-859	787-1031	5.3-12.9	12.0-70
Medium (M)	20-850	$5\ 10^{-5}$	511-681	604-883	8.9-19.6	28-70
~450nm	20-850	10^{-3}	582-710	740-850	11.5-16.0	33-53
Coarse (C)	20-850	$5\ 10^{-5}$	479-701	590-821	11.8-26.4	39-99
700 nm	20-850	10^{-3}	588-712	698-899	15.5-24.5	59-90

The optimal neural network architecture used in this study, including inputs and output (target), is shown in Figure 1.

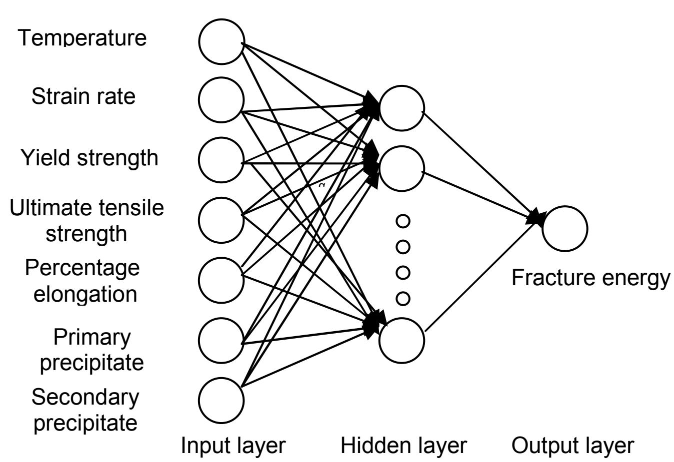

Fig 1: Neural Network Back Propagation Architecture

The MATLAB Neural Network Toolbox is used for optimization of the neural network architecture. Both input and target data are normalized before training to get efficient results. The Trainlm training function which corresponds to the

Levenberg-Marquadt algorithm is used to train the network. The network is trained with 32 data points in total, e.g. 8 data points for each fine, duplex, medium and coarse γ' precipitate structure. For each structure, half of the data are for the low and half for the high strain rate To avoid over fitting, as explained above, total data are divided into three parts: the training (16 data points), the validation (8 data points) and the testing (8 data points). The error goal is set to zero and the network is trained until the actual minimum error is obtained. Once the model is well converged i.e. the error is minimum, the testing data subset results are compared to corresponding experimental values at both strain rates for all precipitate microstructures.

4. Results and Discussions

The final network architecture consists of three layered feed forward back propagation neural network with one input layer, one hidden layer and one output layer. After a number of trials, the most suitable architecture obtained is 7-11-1, which means 7 neurons in input layer, 11 neurons in hidden layer and one neuron in output layer. Fig. 2 shows curves for the convergence characteristics of training, validation and testing data subsets, respectively. The performance is $1.63417e^{-021}$ which is almost close to zero goal.

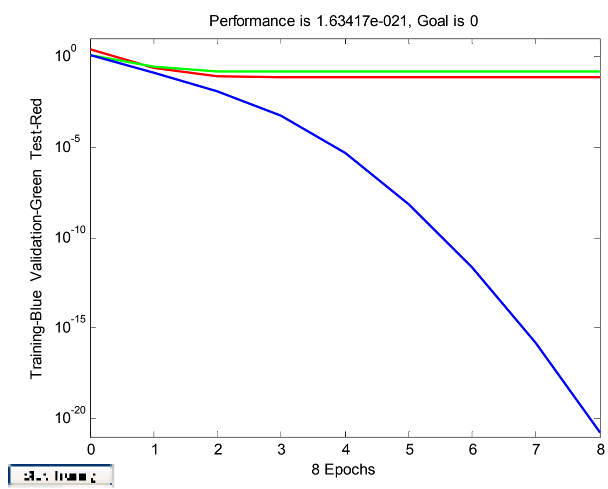

Fig 2: Convergence characteristics of training pattern.

Fig. 3 is the mean squared error vs. epoch curves for training, validation and testing data subsets, respectively. Initially, the mean squared errors for both training and validation data decrease and then becomes constant and the training stops at 8 epochs. It can be seen from this figure that the testing curve also follows the same pattern, which indicates that no overfitting occurred and the network is properly trained.

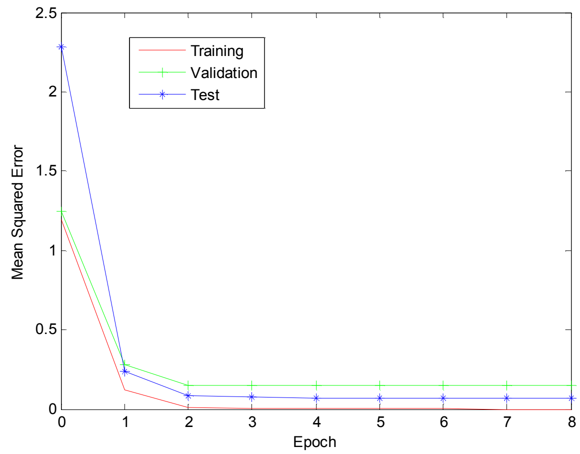

Fig 3: Mean Squared Error for training, validation and testing data subsets

As the model is well developed, model outputs (testing results) are compared with measurement data (fracture energy). Fig. 4 and 5 show a very good match between measurement data and the modeling results at low ($5\ 10^{-5}\ S^{-1}$) and high ($10^{-3}\ S^{-1}$) strain rates, respectively. Data for all precipitate structures, fine (F), duplex (D), medium (M) and coarse (C), are summarized in both figures. This excellent modeling result opens new potential in design and assessing performance and damage of critical components. Due to existing direct correlations between fracture energy, γ' precipitate structure and failure mode, the model can not only be used to assess material strength and toughness, but also to predict the failure mode.

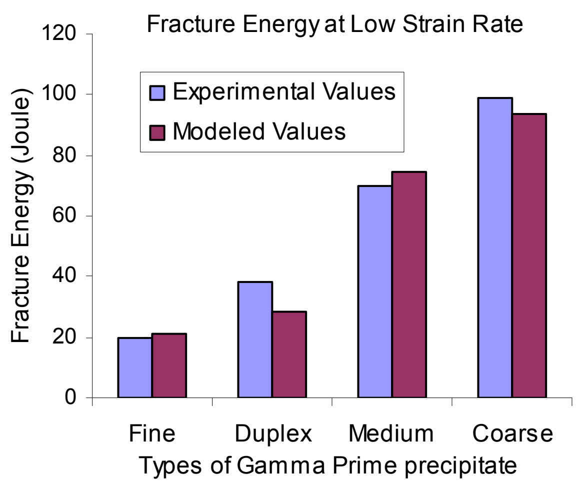

Fig 4: A chart for fracture energy at ($5\ 10^{-5}\ S^{-1}$) strain rate.

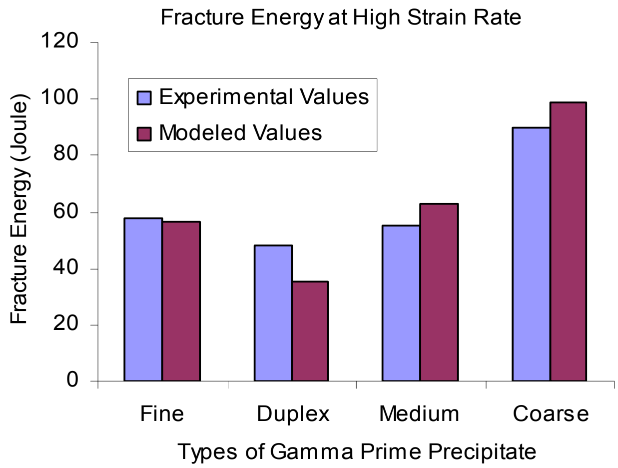

Fig 5: A chart for fracture energy at (10^{-3} S^{-1}) strain rate.

5. Conclusion

A new model based on feed forward Levenberg-Marquadt back propagation neural networks is successfully applied to IN738LC to determine the fracture energy. The proposed model uses application temperature, strain rate, microstructure and common mechanical properties such as yield strength, ultimate tensile strength and percentage elongation to failure as inputs. The neural network results are very consistent with the actual fracture energy values obtained from experimental measurements. As the fracture energy can be directly related to γ'particle structure and failure mode, the model can also be used to predict the failure mode of components.

6. References

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