

THE APPLICATION OF NEURAL COMPUTING METHODS
TO THE MODELLING OF FATIGUE IN NI-BASE SUPERALLOYS

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Abstract

The current financial climate is driving a move towards increased use of computer modelling techniques in alloy design and development in order to reduce cost. In this paper the potential for use of neural computing methods in the prediction of fatigue resistance in Ni-base superalloys is assessed. Initial work has been conducted on the Stage II (Paris regime) behaviour, as the literature indicates that this is the simplest region of the fatigue crack growth curve to predict, with an approximately linear relationship existing between $\log(da/dN)$ and $\log(\Delta K)$, and the crack growth rates being principally affected by temperature, Young's modulus and yield strength. These three parameters were chosen for initial data collection and modelling. The predictions made are of fatigue life, calculated from the slope and intercept values of the linear portion of the log-log fatigue crack growth curve. A test dataset has been successfully predicted along with the trends in the data. The effect of adding ultimate tensile strength and electron valencies as inputs to the model is assessed. It is shown that validation of models produced against metallurgical experience, and careful construction of the database are important conditions for effective use of neural network models for fatigue life predictions.

Introduction

In recent years there has been an increased interest in the ability to model the mechanical properties of alloys from compositional and processing data in order to reduce the cost and time required for alloy development. Increased expectations of engine performance, in terms of speed and range, have led to the need for higher performance alloys, while the financial climate has forced a reduction in the cost of new products.

Good fatigue crack growth resistance is an essential property for superalloys operating in the high temperature stage of gas turbine engines; hence over the last thirty years many studies on the fatigue crack growth behaviour of Ni-base superalloys have been conducted. The general trends in fatigue crack growth behaviour with variations in test conditions (load ratio, temperature and environment), microstructure and processing route are well established. In general such alloys exhibit two stages of long crack fatigue behaviour: Stage I faceted crack growth, occurring along crystallographic {111} planes corresponding to persistent slip bands; and more homogeneous Stage II crack growth resulting in essentially flat fracture surfaces [1]. Inspection intervals for turbine components are often determined on the basis of Stage II fatigue crack growth rates, assuming an initial crack length equal to the smallest detectable flaw size. Such flaws might be surface scratches, coating cracks or casting defects such as pores. In this paper Stage II crack growth is concentrated on as the regime of most interest with respect to lifing procedures.

The fatigue process is sufficiently complicated that, in spite of all the work which has been undertaken in this area, a comprehensive fundamental behavioural model is lacking. Hence a reliable empirical method for predicting fatigue life, using existing data, remains a desirable goal.

The complexity of the fatigue process and the noise associated with fatigue test results has meant that even traditional empirical methods, such as regression analysis, have failed to produce a sufficiently comprehensive, robust model which accurately predicts trends in the data and yet does not model the noise.

Artificial neural networks are powerful computing devices designed to mimic the structure and learning capabilities of the brain, consisting of a large number of simple computational elements (or nodes) which are extensively interlinked via weighted connections. Such networks have the ability to learn rather than being programmed, can pick out complex patterns or trends in data, and can deal with noisy or irrelevant data points in an input dataset. In this paper the possibilities for using such a neural network as a tool to model fatigue using existing fatigue crack growth data are evaluated.

Neural Networks

Artificial neural networks are computational tools based on the structure and function of the brain [2]. They are composed of simple computational elements (called neurons or nodes) which imitate the most basic function of a biological neuron. These artificial neurons are then connected to others by a series of connections broadly analogous to, although much simpler than, those in the brain. The nodes are arranged in layers, with each node being connected to every node in the adjacent layers (figure 1). The simplest node sums N weighted inputs, performs a non-linear function on the sum, and then passes the result to the nodes in the next layer [3]. Data flow forwards only through the network.

There are two phases in the development of a neural network model [4]. Initially the network is 'taught' using a number of example datasets - this process is referred to as training. The training datasets consist of a series of inputs paired with the corresponding output (the 'target' output). An input dataset is applied, the network calculates an output and compares it with the target. The error between output and target is calculated, and the weights in the network are then adjusted using an algorithm (in the case of the network used in this work, a 'back propagation' algorithm) in order to improve the output. The data are fed through repeatedly until the network output is deemed sufficiently accurate (the solution has 'converged'). After this training the network is tested on a set of previously unseen data.

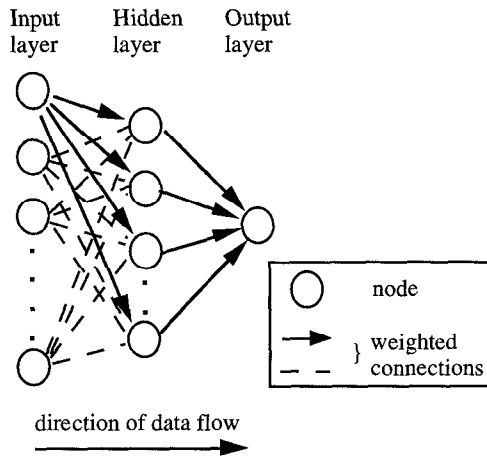


Figure 1 - Schematic diagram of a neural network

It is possible to vary the number of nodes in the hidden layer of the network (the 'architecture'), and care must be taken when deciding the network architecture, as it is possible to overmodel or undermodel the data. If too complex a network is chosen, then the training data will appear to be excellently modelled, however the network will be modelling the noise in the data as well as the trends, so that when the model is tested it will not be robust enough to cope with the new data presented to it. On the other hand, if too simple a network is chosen it will fail to model the trends in enough detail, and predictions will again be very inaccurate. Examples of this type of behaviour are shown in figure 2. In this work, therefore, the network is trained over a number of different architectures and the results are compared.

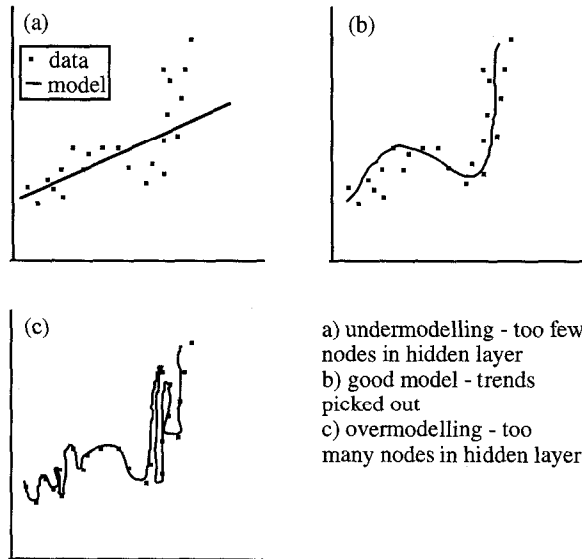


Figure 2 - the effect of number of nodes on modelling accuracy

A point to note is that a neural network learns from experience, and hence while it may interpolate between data with some confidence, it cannot accurately extrapolate into regions for which it has no information, and any attempts at such predictions should be treated with extreme caution.

The main advantage of neural networks over conventional regression analysis techniques is that the network finds an optimum solution without the need to specify the relationships or the form of

relationships between variables. The ability of networks to generalise and find patterns in large quantities of often noisy data is also a major advantage. However the number of sets of training data required to establish a robust network is dependent on the number of input variables (the 'dimensionality' of the data). Previous studies have suggested that the size of the training data should be between three and ten times the input dimensionality[5].

Neural networks in materials science

It has been demonstrated in the literature that neural networks may be used with some success to model material properties and material behaviour [6, 7, 8, 9]. While it is acknowledged that material behaviour is best understood by carrying out experimental programmes, it is not always possible to describe the behaviour in terms of a simple mathematical expression, and hence quantitative modelling of behaviour is difficult, and will become more so as modern materials are further developed with increasingly complex behaviour.

Feedforward neural networks can be very useful in picking out patterns of behaviour and property relationships from a quantity of experimentally produced data, and their ability to generalise can make them useful in predicting the behaviour of a potential new material before it is made. Work on the strength properties of Ni-base superalloys [6] has shown that trends in behaviour with varying composition, temperature and material condition can be modelled, and within error limits absolute values of strength may be estimated.

This paper describes work carried out on the modelling of the Stage II fatigue properties of such alloys using a supervised feedforward neural network as described above.

The datasets

A number of input variables have been considered for presentation to the network. These are: temperature, yield stress, Young's modulus, ultimate tensile strength and Nv number.

Sixty-four sets of input data were gathered from a Rolls-Royce database [27], for which fatigue tests are conducted at a frequency of 0.25 Hz using a 1-1-1 trapezoidal wave form. The network trained using 34 sets and tested itself on the remaining thirty sets.

Before presentation to the network the data for each input variable was normalised between -0.5 and +0.5, according to the equation:

$$n_i = \frac{(x_i - x_{min})}{(x_{max} - x_{min})} - 0.5 \quad (1)$$

where n_i is the normalised value of datapoint i and x_i , x_{max} and x_{min} are the actual values of datapoint i , and the maximum and minimum valued datapoints. This is to prevent a variable from swamping the network simply by virtue of having a large absolute value rather than as a result of the effect of its variation on the result.

Each set of input data is presented to the network along with a corresponding expected output. In this case the chosen output was a 'life' calculated from crack-C and crack-n values where crack-n is the slope of the log da/dN vs. log ΔK fatigue curve in the Stage II region and crack-C is the intercept of this line on the da/dN axis (see figure 3). All fatigue data were produced at a load ratio $R=0.1$, and lives were calculated using a prediction program for a semi-elliptical crack [10]. These 'life' values were also normalised.

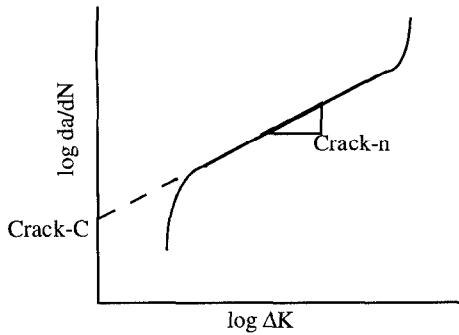


Figure 3 - Schematic to show crack-C and crack-n

When choosing a dataset to train the network on it is important to try and ensure that the data are spread evenly over the areas of input space which are of interest. Otherwise the network may be attempting to extrapolate from well defined regions of input space into regions about which nothing is known, and predictions may be unreliable. The range of values of input and output data is shown in figure 4.

Training and testing the network

The network used is based on a Bayesian statistical framework, which allows the probability of a model being a true representation of the data to be assessed[11]. Initial weights are set using a

random number generator which is started using a 'seed'. This seed can have any positive value, and using different seeds may produce slightly different models. In order to ensure that all potential model types are generated the network is trained using a number of seed values for each architecture.

The network finds the optimum solution by minimising a penalised likelihood, in effect trying out a number of solutions to find the best relationship. As well as calculating the weights for the connections the network calculates a number of other parameters:

σ_{nu} - a measure of the noise allowed in the network's prediction of the data. Initially this is set at a fairly large value, and the program modifies the inferred noise level as it develops the model to more accurately fit the data. The value of this parameter varies with the number of nodes, generally decreasing to a limit as the number of nodes increases and a more complex model is formed such that the relationship between inputs and outputs is better modelled. The value of σ_{nu} is a fraction of the range of the output data, e.g. $\sigma_{nu}=0.2$ means that the inferred noise in the data is 20% of the range of the target output dataset.

training energy - a measure of the error in predicting the training dataset targets (this usually follows a similar pattern to σ_{nu}).

test energy - a measure of the error in predicting the previously unseen test dataset. This initially decreases with increasing number of nodes to a point, but if overmodelling starts to occur, and the network has effectively 'learnt' the training dataset, then it will be unable to cope with noise in the test set and test energy will start to increase.

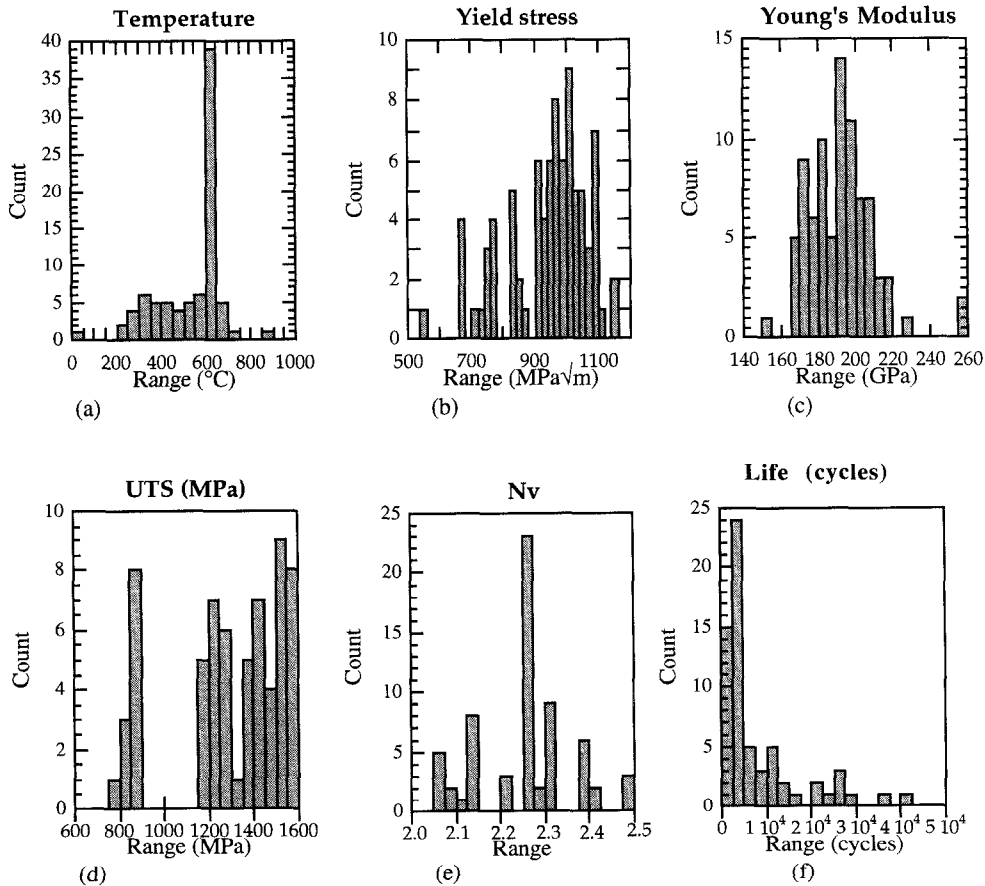


Figure 4 - graphs to show the range of the input and output data

relevance - this is a value which is produced for each input to the network, and is a measure of how important that input is in the model produced. A highly important input would have a relevance of the order of 1, whereas an input which is perceived to be irrelevant would be assigned a relevance of the order of 10^{-3} or less.

Energy values are calculated from the following equation:

$$energy = \frac{1}{2} \sum (o - t)^2 \quad (2)$$

where o is the output value and t is the target value.

In order to be useful as a cost-saving design tool, the number of inputs to the network should ideally be kept to the minimum possible. For this reason it was decided to 'start small' and present the network with few variables, gradually adding other possibly important variables to see whether they had a positive or detrimental effect on the predictive ability of the network. Another advantage of this approach is that it keeps the input dimensionality low, thus requiring less data to produce a robust model.

The basic database

A review of literature on Stage II Paris regime fatigue crack growth and crack tip opening displacement (CTOD) models for crack growth indicates that the most important properties affecting fatigue crack growth are likely to be yield strength and Young's modulus [12, 13, 14, 15, 16, 17, 18, 19]. CTOD theory suggests the following form of equation for fatigue crack growth rate:

$$\frac{da}{dN} \propto \frac{\Delta K^2}{\sigma_{ys} E} \quad (3)$$

where da/dN is the crack growth rate, ΔK is the stress intensity factor range, σ_{ys} is the yield stress and E is the Young's modulus [17, 18]. The literature also suggests that test temperature is an important factor affecting fatigue crack growth rates [20, 21]. Hence initial modelling used an input dataset consisting of temperature, σ_{ys} and E .

The network was trained for 2-8 hidden nodes. For each number of nodes seeds of 0, 20, 40, 60 and 99 were used.

A plot of σ_{nu} vs. number of nodes is shown in figure 5a. Two different types of model are generated by the network, depending on the initial random weights (determined by the 'seed'). The first type tend to have relatively high σ_{nu} values (0.18, or 18% of the range of the output data), this value being independent of the number of nodes. This indicates that an over-simple model is being produced which is just as accurately described with two nodes as with five or seven. Training and test energies for these models followed a similar pattern and were also high, with values of about 0.5 in both cases. This type of model will be referred to as the simple model.

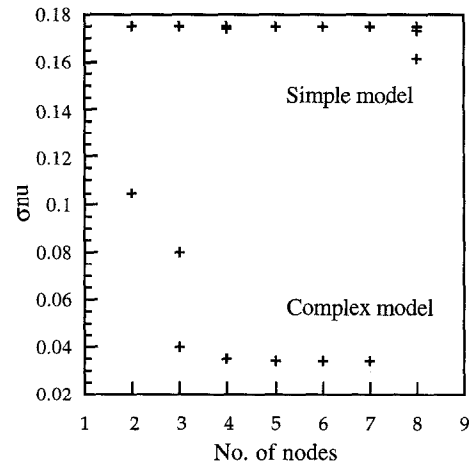


Figure 5a) - Graph of noise vs. no. of nodes for the simple dataset

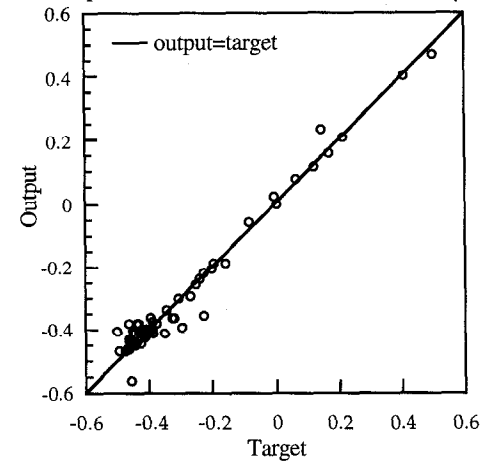


Figure 5b) - Graph of network output vs. target output for a type-B model

The second set of models on the other hand display a decreasing noise level, reaching a minimum of about 0.034 at four hidden nodes, indicating the formation of a more complex model. Training and test energies again followed a similar pattern, with values of training energy around 0.015 and test energy around 0.03. When the relevance values of the input variables for the two different types of model were compared it was found that the simple models all had very low relevance for Young's modulus (e.g. $1 \cdot 10^{-4}$, c.f. 0.6 for yield stress) whereas the more complex models attributed a much higher relevance to Young's modulus (e.g. 1.4, c.f. 2.2 for yield stress), more in accordance with CTOD theory and experimental evidence. A graph of predicted output vs. target output for a complex model is shown in figure 5b. It can be seen that predictions are good, with most of the predictions lying very close to the line for output = target.

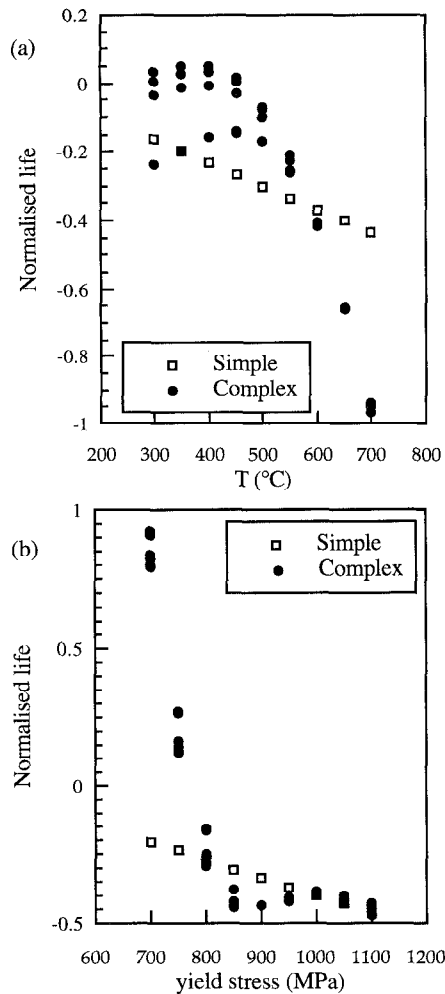


Figure 6 - Predictions of life generated using the simple database for (a) varying temperature and (b) varying yield stress

It is important to test the physical validity of a neural network model, to ensure that the network really has converged, and has not found a local minimum in the data. Thought experiments were conducted using a model dataset in which the input variables took on the median value of the original dataset ($T=600\text{ }^{\circ}\text{C}$, $\sigma_{\text{ys}}=950\text{ MPa}$, $E=195\text{ GPa}$) and then each variable in turn was varied in order to see what trends the neural network had found. The best six complex models, ranked on test error, were chosen and the best simple model was used for comparison. The prediction of life with variation in temperature is shown in figure 6a. The prediction follows the expected trend of decreasing life with increasing temperature [21], with the effect becoming more marked as temperature increases. This can be understood both in terms of the decrease in yield stress (typically about 10% for a given alloy over this temperature range) and also the likely change in deformation mechanism. At higher temperatures a transition from planar to wavy slip is expected, with increased cross slip occurring and slip becoming inherently less reversible, resulting in more damage accumulation per cycle. The simple model produces a much simpler linear trend, indicative of undermodelling. The prediction of life variation with Young's modulus for the complex models shows a roughly linear increase in life with increasing Young's modulus, in accordance with what might be expected from CTOD theory and from experiment [22], while the simple models show life to be independent of E , as would be expected from the low relevance assigned to it.

When predictions of varying yield stress are examined, however, an unexpected result is obtained, as life is predicted to decrease rapidly as yield stress increases from 700-800 MPa, followed by a slight increase to 1000 MPa and then a further gentle decrease in life (figure 6b). CTOD theory on the other hand would indicate an increase in life with increasing yield stress in a similar manner to that seen in the Young's modulus predictions. There are two possible reasons for this apparent anomaly. It is possible that it may be explained by the fact that these predictions were made for a temperature of $600\text{ }^{\circ}\text{C}$, and the data contain only two alloys with a yield stress less than 800 MPa at this temperature, both of which have a Young's modulus of about 170 GPa, rather than the 195 GPa used for prediction. Hence attempting to predict life in the data range used may effectively be an extrapolation into an unknown area. While such extrapolations may not necessarily be totally misleading, this example illustrates that care is needed if attempting them. It also indicates the importance of constructing, where possible, a database which would cover the possible range of data of interest if neural network modelling is to be used as a design tool. That is not to say however that a neural network could not be used to reduce experimentation - if an unexpected result is found, then one or two experiments in the area of interest may suffice to test the proposed model, without an entire test matrix being required. The results could then be added to the training dataset.

Another possible explanation is revealed by further examination of the input data. If the data for life are plotted versus yield stress for temperatures between $550\text{ }^{\circ}\text{C}$ and $650\text{ }^{\circ}\text{C}$ (figure 7) it can be seen that there is in fact a reduction in life with increasing yield stress at low yield stress ranges. The points which cause this are all points for one particular alloy in the database which is a casting alloy, as opposed to a wrought alloy, and hence has a very different microstructure compared to the other alloys in the database. Examination of the actual test data revealed that the tests had been conducted on specimens containing only two grains, and the cracks had deflected at high angles from the normal to the principal stress, giving low apparent crack growth rates. The existence of only two grains in the specimens and the high deflection angle of the cracks indicate that the cracks may have propagated in Stage I, where CTOD models do not apply, as slip is inhomogeneous, being concentrated in intense bands. The low crack growth rates may have occurred as a result of crack closure [21] and/or shielding due to crack deflection [26], both of which reduce the effective stress intensity at the crack tip. This result indicates the importance of careful construction of the database to cover the problem of interest, without including spurious data.

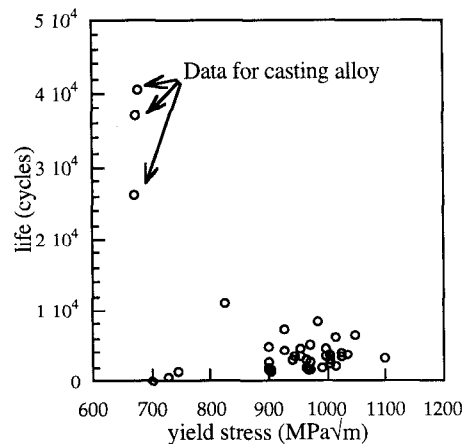


Figure 7 - Life versus yield stress for all data in the temperature range $550\text{--}650\text{ }^{\circ}\text{C}$.

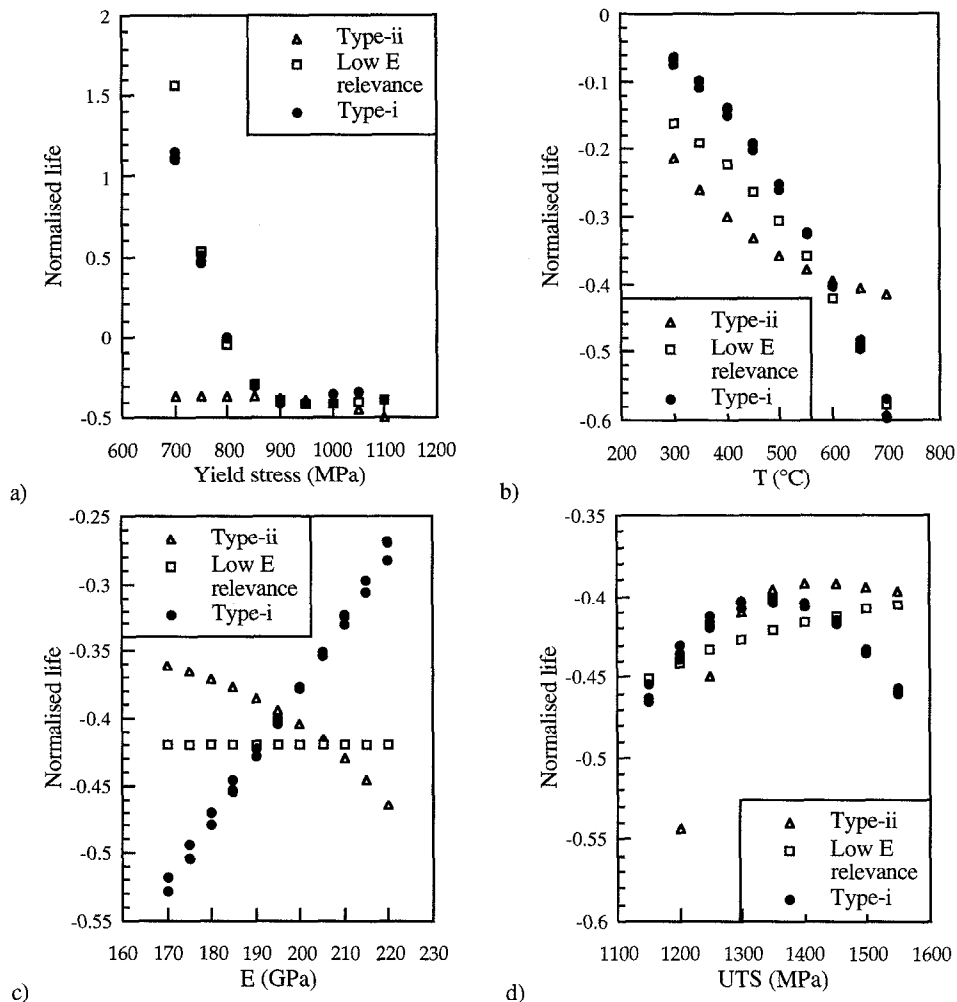


Figure 8 - Predictions of life generated using a database containing UTS for (a) varying yield stress (b) varying temperature (c) varying Young's modulus (d) varying UTS

Refining the data base

The model produced so far has been somewhat simplistic, with only three input variables used, and while some success has been obtained it was thought useful to add further parameters to see whether network performance improved. However, collecting data can be problematic as in order to use a given dataset it is necessary to have values for all the inputs. It would have been informative to look at grain size and other microstructural parameters, as Stage II fatigue is expected to be microstructurally sensitive to some extent [20]. Unfortunately, microstructural information is difficult to obtain from reports, papers and standards to a sufficient degree of accuracy to be useful in the network. Hence material property data and such data as are calculable from thermodynamic phase calculation programs such as MTDATA are used as inputs, as these are more readily available/determinable.

Accounting for cyclic hardening

In equation 3, the yield stress in the denominator is that at the crack tip. This may or may not be similar to the bulk yield stress, as repeated yielding of material in tension and compression may cause cyclic hardening or softening. Hence the cyclic yield stress may differ from the bulk yield stress. Data for cyclic yield stress are not readily available. However Manson and Hirschberg [23] proposed

an empirical relationship between 'hardenability' and the ratio of ultimate tensile strength (UTS) to yield stress. Materials with a ratio greater than 1.4 are proposed to cyclically harden, those with a ratio less than 1.2 to cyclically soften, and those with a ratio between 1.2 and 1.4 to be cyclically stable. Therefore UTS was added to the database as an input to the network to provide a measure of deformation characteristics.

The addition of UTS as an input produced three types of low noise models, which had comparable noise levels and training and test energies to those produced previously. In this instance a number of the models (about half) assigned a low relevance to E . Of those that did not, again the best six models were chosen, ranked by test error, and were then compared with a model with low relevance for E . When predictions of variation in life with yield stress are made (using a mean UTS value of 1360 MPa), it may be seen that the models fall broadly into two groups, those that predict a large drop in life with yield stress increasing from 700-800 MPa (type-i) and a group which indicates a more linear dependence of life on yield stress (type-ii) (figure 8a). Above 800 MPa the two sets of models agree reasonably well. While the type-ii models at first seem promising, examination of predictions for temperature and Young's modulus calculation cast doubt on their validity (figure 8b & c). The prediction of temperature dependence shows a different form from previous models, and indicates a lessening of the effect of temperature as temperature increases, whereas observations on increased dislocation mobility with temperature would indicate an

increasing effect of temperature as demonstrated by type-i. Dependence of life on Young's modulus for type-ii models is the reverse of that predicted by CTOD theory and experimental observation.

The dependence of life on UTS is shown in figure 8d. The type-i models predict an evident but modest dependence of life on UTS, indicating some importance of UTS, although it seems less important than temperature and E . The type-ii models however indicate a strong dependence of life on UTS below about 1250 MPa, above which value the two types of model agree reasonably well. When the values of predicted life are examined it is noted that below 1250 MPa the values fall well outside the range of the dataset (-0.75 as opposed to a limit on the data of -0.5). Again it is possible that the model is trying to extrapolate too far from the known database, and so such predictions should be regarded with care, as in the case of the yield stress predictions described above. Examination of the database reveals that at 600 °C the alloys with low UTS also have very low Young's modulus (about 170 GPa as opposed to the value of 195 GPa used for predictions).

Of the three models, type-i best reflects the actual trends in the data. The existence of two complex models with low noise and test energy indicates that within the experimental noise in the data there is more than one way to mathematically model the data. However, only one of these models makes physical sense. This difference in prediction by two sets of models which are ostensibly similar shows the importance of thoroughly examining a neural network model in the light of metallurgical knowledge.

The effect of alloy instability

It has been observed that some alloys which are unstable to the formation of the detrimental sigma phase have an increased resistance to fatigue crack propagation [24]. It is possible to express this instability in terms of an electron valency number (N_v) of the matrix, which can be readily calculated from alloy composition [25]. This parameter, N_v , was used as an input to the network in order to investigate this dependence. N_v has the advantage, along with yield stress, of being a means of entering compositional information without needing to enter the composition itself (which would vastly increase the input dimensionality and hence the number of datasets needed to produce a robust model).

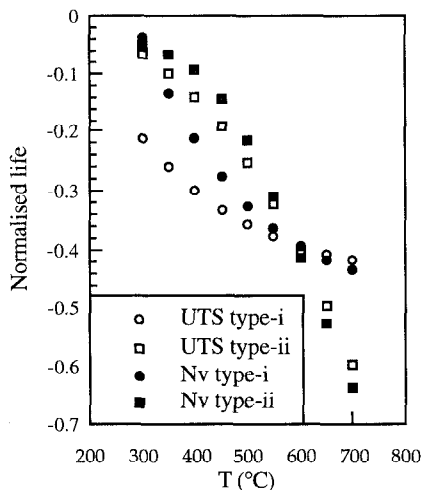


Figure 9 - comparison of predictions using data-base containing UTS and database with N_v added

Addition of N_v to the database again produces two types of complex model, similar in form to those described above (e.g. figure 9, $N_v=2.27$). The relevance attributed to N_v is quite high, and life is predicted to increase roughly linearly with N_v by both models (figure 10). The difference in life is not predicted to be very large as the range of N_v values in the database is quite small. This indicates that, although there is an effect of N_v on fatigue resistance, the benefits obtained by trying to alter N_v within the Ni-based alloy system would not be great as this class of alloys tends to exhibit a restricted range of N_v values.

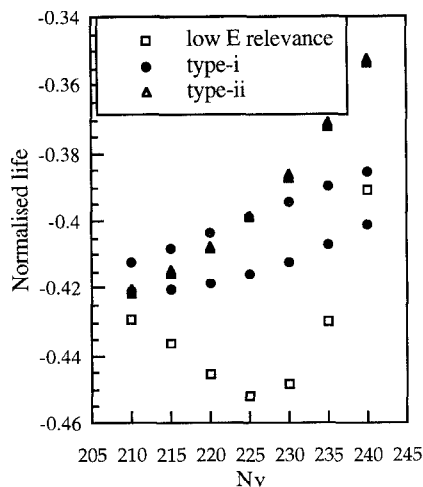


Figure 10 - Prediction of variation of life with N_v

Summary and Conclusions

A possible limitation on use of neural networks as predictive tools for design purposes is the amount of data required - large numbers of inputs require large, complete datasets which are difficult to compile. However success has been achieved in modelling Stage II fatigue crack growth behaviour in Ni-based superalloys. A basic dataset containing temperature, yield stress and Young's modulus models trends adequately, while refining the database to include ultimate tensile strength improves the performance.

The importance of careful construction of a database has been stressed, in order as far as possible to cover areas of input space that may be interesting, as extrapolative predictions must be treated with caution. Experimental results that may be of use in a database should be carefully logged to ensure that relevant inputs, such as microstructural information, are recorded accurately. It has been seen that it is important to validate any neural network model produced to ensure that its predictions are in line with experience.

It has been shown that it is possible to use a neural network to investigate and model trends in fatigue crack growth behaviour with variation in material properties, based either on proposed mechanisms or on observed empirical trends. A trend for increased Stage II fatigue life with increased instability to sigma-phase formation (indicated by electron valency number, N_v) has been shown to exist, although the observed effect is small due to the small range of N_v in Ni-based superalloys.

While further work on validation of such networks is required before they can be used in design, if such work is done neural networks may prove to be of great benefit in future alloy design programmes.

Acknowledgements

Professor C.J.Humphries is thanked for provision of research facilities at the University of Cambridge. Rolls-Royce plc are thanked for financial support for this work and for the provision of data. Thanks are also due to Joy Jones of the University of Cambridge for helpful discussion and advice.

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