Final Report GR/K23263
Quantitative Alloy Design Tools for Ni–Base Superalloys

INTRODUCTION & ORIGINAL OBJECTIVES

Alloy design for critical aeroengine components such as turbine blades and discs is a difficult, time–consuming and expensive process. The development period prior to application in an engine is typically of the order of ten years. Airframe manufacturers usually announce a new design only five years prior to flight certification. This leaves the engine designers only half the current period necessary for materials development.

Despite decades of research on the γ/γ' nickel base superalloy system, new alloys have in the past been investigated by making as many as a hundred different variants. Each of these has to be cast or made into powder form, thermo–mechanically processed, assessed for the presence of deleterious phases and for processability, and tested on a laboratory scale. There is a further stage of optimisation before a small selection of alloys is tested to commercial standards. Predictive modelling, at any stage of this empirical alloy design procedure, would obviously reduce the cost and the time involved in the development of new materials. It was the intention of this project to create some of the tools needed for the modelling of nickel–base superalloys.

The objectives as listed in the original proposal are as follows:

1. To develop quantitative strength prediction models γ/γ' Ni–base superalloys.
2. To develop quantitative models for other mechanical properties, particularly fatigue
3. To produce these models in the form of usable alloy design tools.

We shall now describe the range of models that has been developed in order to enable weld design.

SOLID SOLUTION STRENGHTENING OF γ

Nickel base superalloys are essentially mixtures of γ' precipitates ($L1_2$ structure) in a disordered γ (cubic–close packed structure) matrix. The yield strength of multicomponent nickel solid solution alloys has not been modelled in the past with respect to the effects of temperature and chemical composition. There have been investigations of the effect on the yield stress of solutes in binary systems at a fixed temperature, but not for multicomponent solutions or as a function of the test temperature. Solid solution theory has been used to solve this [1].

Two forms of the "trough" model, in which dislocations reside in energy wells, were used to determine the most appropriate model. The yield strength of three binary nickel–chromium and three ternary nickel alloys were determined experimentally over a range of temperatures. The data were then modelled using the Feltham equation (a trough model). The constants determined by fitting the Feltham equation to the experimental data were then applied to other experimental solid solution alloys and also to published information on commercial solid solution nickel alloys. It was thus demonstrated that the yield strength of γ solid solutions can be modelled successfully using the Feltham equation [1].

THE NEURAL NETWORK METHOD

Many mechanical properties are so complex in their dependance on material characteristics that there are no theories available to make quantitative predictions of the kind necessary in engineering design. The neural network method is ideal in such circumstances since it thrives in complexity, and when combined with experience from physical metallurgy, can be enormously useful both in the design of new materials and in the definition of critical experiments.

Neural networks are parameterized non–linear models used for empirical regression and classification modelling. Stated simply, this represents a method for the quantitative recognition of patterns in data, without any *a priori* specification of the nature of the relationship between the input and output variables. They can model relationships of almost arbitrary complexity.

The outcome of neural network training is a set of coefficients (called weights) and a specification of the functions which in combination with the weights relate the input to the output. The training process involves a search for the optimum non–linear relationship between the inputs and the outputs and is computer intensive. Once the network is trained, estimation of the outputs for any given inputs is very rapid.

There are methods, such as that of MacKay [2], which implement a Bayesian framework on the neural network; this helps in the determination of the relevance of individual inputs. Furthermore, the error bars then depend on the specific position in input space, reducing the dangers of extrapolation and interpolation. These methods and associated references are described fully in [2]. We have found throughout the present work that the method is capable of revealing interesting metallurgical trends.

OVERALL STRENGTH

The yield and ultimate tensile strength of nickel–base superalloys with γ/γ' microstructures has been modelled [3,4] using the neural network method, as a function of the Ni, Cr, Co, Mo, W, Ta, Nb, Al, Ti, Fe, Mn, Si, C, B, and Zr concentrations, and of the test temperature. The analysis is based on data selected from the published literature. The trained models were subjected to a variety of metallurgical tests. As expected, the test temperature (in the range 25–1100 °C) was found to be the most significant variable influencing the tensile properties, both via the temperature dependence of strengthening mechanisms and due to variations in the γ' fraction with temperature. Since precipitation hardening is a dominant strengthening mechanism, it was encouraging that the network recognised Ti, Al and Nb to be key factors controlling the strength. The physical significance of the neural network was apparent in all the interrogations we performed.

One example illustrating this last point is presented in Fig. 1. The softening of the γ matrix is offset by the remarkable reversible increase in the strength of the γ' with increasing temperature.

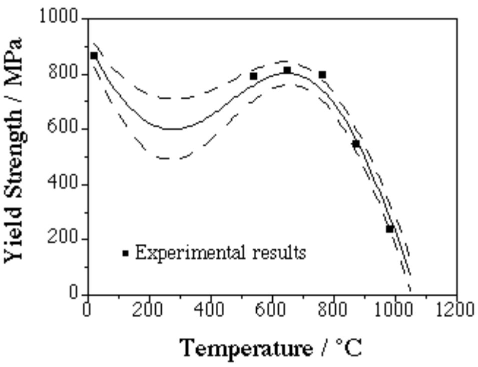

Fig. 1: Predicted temperature dependence of the yield strength of a γ/γ' superalloy.

A further revelation from the neural network analysis came from the error estimates, which demonstrated clearly that there are great uncertainties in the experimental data on the effect of large concentrations of molybdenum on the tensile properties. This has identified a region where careful experiments are needed; these will be conducted in future studies since molybdenum is known to have a large influence on the γ/γ' lattice misfit.

The methodology for tensile properties has already been exploited in Rolls–Royce to reduce the number of variants involved in experimental alloy design programmes.

FATIGUE PROPERTIES

An extensive literature review was carried out to assess methods for predicting the fatigue crack growth rates. Physical models were examined but where either found not to be generally applicable or gave only qualitative indications of the trends [5]. Selected experiments were conducted [6] to clarify the factors controlling the initiation and propagation of cracks in turbine–disc superalloys. These results failed to clarify how fatigue theory could be used to make quantitative predictions.

A neural network method was therefore used after identifying some 51 variables that could be expected to influence the fatigue behaviour of nickel base superalloys [7]. The variables included the stress intensity range ΔK, chemical composition, temperature, grain size, heat treatment, frequency, load waveform, atmosphere, R–ratio, the distinction between short and long crack growth, sample thickness and yield strength. The analysis was conducted on some 1894 data collected from the published literature.

The model, unlike any experimental approach, could be used to study the effect of each variable in isolation. This gave interesting results. For example, it was verified that an increase in the grain size should lead to a decrease in the fatigue crack growth rate, when the grain size is varied without affecting any other input. This cannot be done in experiments because the change in grain size is achieved by altering the heat treatment, which in turn influences other features of the microstructure (Fig. 2). It was also possible to confirm that $\log\{\Delta K\}$ is more strongly linked to the fatigue crack growth rate than to ΔK, as expected from the Paris law. There are many other metallurgical trends revealed [7]. The method has been used in the context of a Rolls–Royce disc alloy development programme, where it was demonstrated quantitatively that the uncertainties of current knowledge are so large that experiments were definitely necessary.

Fig. 2: Astroloy: (a) effect of grain size alone; (b) effect of heat treatment alone [7].

In another approach [8] a different neural computing approach was used to focus on stage II of the Paris regime, where the growth rate should depend mainly on the stress intensity range, Young's modulus and yield strength. The model was used successfully in estimating new test data. The effect of the ultimate tensile strength and phase stability was also investigated; although this proved promising, it is probable that the results will be more convincing when a greater range of data become available.

CREEP

The creep rupture life of nickel base superalloys has been modelled as a function of 42 variables including Cr, Co, C, Si, Mn, P, S, Mo, Cu, Ti, Al, B, N, Nb, Ta, Zr, Fe, W, V, Hf, Re, Mg, La and ThO_2 [9]. Other variables include four heat treatment steps (characterised by temperature, duration and cooling rate), the sample shape and the solidification method.

The results have been interpreted using physical metallurgy principles where this is possible, and the model is currently being used in our Technology Foresight Programme.

LATTICE PARAMETERS

The lattice constants of the γ and γ' phases of nickel superalloys have been modelled using a neural network within a Bayesian framework [10]. The analysis was based on new X–ray measurements and peak separation techniques, for a number of alloys and as a function of temperature. These data were supplemented using the published literature.

The lattice parameters of the two phases were expressed as a non–linear function of eighteen variables including the chemical composition and temperature. It was possible to estimate the uncertainties and the method has proved to be extremely useful in understanding both the effect of solutes on the lattice mismatch, and on how this mismatch changes with temperature. The method has been used in the development of new single–crystal alloys (TMS series) where rafting is an important phenomenon.

OTHER MATERIALS & PROCESSES

Our experience with neural networks has been very positive so the method has been applied outside of the scope of the original project.

The treatment of iron–base superalloys using both neural network and physical modelling is described in [11,12]; a description of the modelling of constitutive relations obtained by torsion testing is in [13]; the modelling of steel plate processing using more than 100 variables is in [14].

DISSEMINATION

A lot of the work and data are available from the materials algorithms project world wide web (www) site on

http://www.msm.cam.ac.uk/map/mapmain.html

and specifically on MAP_LATTMISIFT (lattice misfit), MAP_FAT_Ni_MAT (fatigue properties), MAP_STEEL_NEURAL (iron base superalloys), MAP_NEURAL_MASTEEL (iron base superalloys).

The work, including the weights, has been published widely (see list) and has been presented at a variety of conferences and colloquia.

PUBLICATIONS

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    ISIJ International, Vol. 38 (1998) 495–502.
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11. "Tensile Properties of Mechanically Alloyed Oxide Dispersion Strengthened Iron Alloys. Part 1 - Neural Network Models"
    Materials Science and Technology, Vol. 14, 1998, 793–809.
    A. Y. Badmos, H. K. D. H. Bhadeshia and D. J. C. MacKay

12. "Yield Strength of Mechanically Alloyed ODS Iron Alloys. Part 2: Physical Interpretation"
    Accepted for publication in Materials Science and Technology, 1997
    A. Y. Badmos and H. K. D. H. Bhadeshia
13. "Estimation of Hot Torsion Stress–Strain curves in Iron Alloys Using a Neural Network Analysis"
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    V. Narayan, R. Abad–Lera, B. Lopez, H. K. D. H. Bhadeshia and D. J. C. MacKay
14. "Neural Network Analysis of Steel Plate Processing"
    Accepted for publication in Ironmaking and Steelmaking, 1998
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SUMMARY

Introduction:

The development of new nickel alloys for aeroengine applications is a difficult taks, frequently achieved by trial and experience. The purpose of this work was to enable a significant proportion of the development procedure to be done by computation. A variety of methods have been used towards this end, ranging from physical models to the power technique of neural network analysis.

A more general method of regression is neural network analysis. As before, the input data x_j are multiplied by weights, but the sum of all these products forms the argument of a hyperbolic tangent. The output y is therefore a non–linear function of x_j, the function usually chosen being the hyperbolic tangent because of its flexibility. The exact shape of the hyperbolic tangent can be varied by altering the weights. Further degrees of non–linearity can be introduced by combining several of these hyperbolic tangents, so that the neural network method is able to capture almost arbitrarily non–linear relationships. For example, it is well known that the effect of chromium on the microstructure of steels is quite different at large concentrations than in dilute alloys. Ordinary regression analysis cannot cope with such changes in the form of relationships.

A potential difficulty with the use of powerful regression methods is the possibility of overfitting data. For example, it is possible to produce a neural network model for a completely random set of data. To avoid this difficulty, the experimental data can be divided into two sets, a *training* dataset and a *test* dataset. The model is produced using only the training data. The test data are then used to check that the model behaves itself when presented with previously unseen data.

Neural network models in many ways mimic human experience and are capable of learning or being trained to recognize the correct science rather than nonsensical trends. Unlike human experience, these models can be transferred readily between generations and steadily developed to make design tools of lasting value. These models also impose a discipline on the digital storage of valuable experimental data, which may otherwise be lost with the passage of time.

We have addressed solid solution strengthening, tensile properties, fatigue, creep, lattice misfit in the context of nickel–base superalloys, and have applied the method to other materials and processes.

Achievements: A large number of quantitative models have been produced, dealing with the microstructure and mechanical properties of nickel–base superalloys. This is the first time it has become possible to estimate properties as complex as the fatigue crack growth rate as a function of a very large number of variables. The models have been tested successfully against the known principles of physical metallurgy. They have been used already, both in reducing the scale of experimental programmes and in identifying regimes where experiments are essential.