A predictive model for the anisotropic deformation of a single crystal superalloy has been applied to the alloy SRR99. Model parameters are derived from a database of creep curves. The model predictions are compared with both characteristic shape and crystal rotations that occur during high temperature deformation and with the results of mechanical tests. Model and experiment are shown to agree and exceptions are discussed with respect to macroscopic microstructural features and the operation of cube and octahedral slip systems.

**Introduction**

Single crystal nickel-base superalloys comprise an important class of engineering alloys for high temperature applications. Their primary use in turbine blades relies on their resistance to elevated temperature deformation. In order to exploit fully the creep capabilities of these alloys, both microstructural and engineering approaches must be developed. Even for isotropic materials, generation of a complete database of all types of mechanical behaviour required for design is impractical and crystallographic anisotropy introduces additional complexity. To address the design issues, a unified approach combining engineering modelling backed by an underlying knowledge of the micromechanisms controlling the material behaviour is required if these alloys are to be used to their full potential. Both approaches must be employed to ensure effective extrapolation to conditions not covered by available data; an understanding of the deformation mechanisms and the influence of microstructure must be presented in a form that can be used in the design process, and from the engineering aspect, predictive models for creep performance must be developed to allow full implementation of these alloys in their desired application.

The aim of the present work has been to continue the development, validation and use of a constitutive description of anisotropic creep deformation that can be quantified by the analysis of a limited database of creep tests but is capable of extrapolation to other conditions. The model has built upon previous work based on continuum damage mechanics (1) to represent the deformation rate at any given time in terms of state variables that are related to the mechanisms and microstructural evolution that controls the deformation rate (2, 3). This paper will assess the representation from the anisotropic model of a database of creep for the single crystal superalloy SRR99 and compare the predictions of high temperature behaviour with experimental data. Validation of the model by measurement of changes in crystal orientation using electron back scattering patterns and changes in specimen shape will be summarised. In addition, microstructural variations including those associated with casting porosity and γ' morphology relative to the model predictions will be described.

**Anisotropic Model - Data Analysis**

The model for anisotropic creep used in this study was originally described by Ghosh, Curtis and McLean (4) and its subsequent development has been described in detail elsewhere (5, 6) and are summarised in the Appendix. The approach taken in the present assessment of the model has included prediction of mechanical behaviour as well as of crystallographic and macroscopic geometrical changes in specimen characteristics during deformation. The anisotropic model accounts for the deformation observed in single crystals by restricting deformation to specific slip systems and to occur at a given rate (4). This rate depends on the resolved shear stress, temperature and state variables incorporating damage parameters. Individual creep curves can be used to derive these model parameters as described by Dyson and McLean (3). Data analysis was performed on a data set consisting of uniaxial creep tests for two orientations <001> and <111> of the single crystal superalloy SRR99 conducted by the Defence Research Agency, Farnborough. Tests were at constant stress ranging from 150 to 950 MPa and temperatures were between 750 to 1050°C. Figures 1 and 2 present experimental creep curves for these two orientations. Although all curves show a tertiary creep region, differences in the shape of these curves are apparent such as the limited range of primary creep at 1050°C for both orientations. At lower temperatures, marked differences between the responses of the two orientations can be seen.

![Figure 1: Creep curves for different stress and temperature conditions for <001> oriented specimens of SRR99.](image)
These differences pose a challenge to the data analysis but the model can cope with these variations by using the approach for the derivation of model parameters first proposed by Dyson and McLean (3).

The approach has been to analyse each individual creep curve to determine the optimum set of model parameters. Simple representations of these parameters as a function of stress and temperature were then derived. Figure 3 presents a comparison of the model predictions based on this global parameter set with the entire creep database for SRR99. At temperatures of 750°C, 850°C and generally 900°C, the model predictions show consistency with the experimental data. However, as the temperature increases to 950°C and 1050°C, this excellent agreement between experiment and prediction decreases and may result from the microstructural changes to be described and from alterations in the active slip systems.

**Anisotropic Model - Predictions and Experimental Validation**

Scanning electron micrographs generated using secondary electrons from electroetched specimens showing the typical γ' morphology evolved at 850°C and 950°C are presented in Figure 4. At the lower temperature although the γ' has lost its initial cuboidal shape, it typically exists as discrete particles. As the test temperature increases to 950°C, extensive rafting is observed. This change in precipitate morphology has been proposed to influence the deformation mechanism in superalloys and may account for the model deviations described in the previous section and shown in Figure 3.

**Figure 3a:** Comparison of the measured and predicted times to reach 5% creep strain for <001> specimens of SRR99.

**Figure 3b:** Comparison of the measured and predicted times to reach 2% creep strain for <111> specimens of SRR99.

**Figure 4:** Secondary electron micrographs showing the difference in γ' morphology for a <210> oriented specimen after creep testing at:

(a) 850°C, 550MPa, time to failure 149.5h
(b) 950°C, 300MPa, time to failure 112.5h.
Validation from Macroscopic Measurements of Creep Specimens

As a result of the high levels of creep strain before fracture, the tensile creep specimens are highly necked on failure. Consequently, there is a considerable gradient in local strain as measured by the reduction in area. Macroscopic measurements of deformation such as crystal rotation and changes in specimen shape from the original circular cross-section characteristic of the gauge length prior to deformation provide a challenging test of the model validity. In the latter case, after careful determination of the initial orientation using Laue techniques, diameters of the gauge at various distances along the specimen length were measured as a function of rotation and related to the local reduction in area and to a reference transverse direction on creep fractured specimens that were part of the database. Using the model predictions shown by the uninterrupted line, good agreement with the experimental data is obtained as can be seen in Figure 5. In some cases, such as shown in Figure 6, experiment and model agree only when cube shear is allowed to dominate. This provides strong justification for the initial premise of the model that both cube and octahedral shear can occur. A summary of the observations is presented in Figure 7 indicating that cube shear is restricted to orientations in the vicinity of <111> (7). It must be noted, however, that the summary covers a range of temperatures and does not describe the slip behaviour at a given temperature.

Figure 5: Comparison between the measured and predicted creep specimen cross-section at various levels along the gauge length of a nominal <110> oriented specimen of SRR99. The experimental data are shown on the right, the prediction is shown by the solid lines on the left.

Figure 6a: Comparison of the measured change in specimen shape of a failed creep specimen of SRR99 with a <112> orientation with model predictions assuming only cube slip.

Figure 6b: Comparison of the measured change in specimen shape of a failed creep specimen of SRR99 with a <112> orientation with model predictions assuming only octahedral slip.

Figure 7: Summary of experimental and predicted changes in cross-sectional area for SRR99 creep specimens.
The same specimens were sectioned parallel to the gauge length and the resulting surface was mechanically polished followed by electropolishing in 10% orthophosphoric acid in water. The local orientations were determined along intervals of the length using electron back scattering patterns (EBSP) and in some cases, a matrix of orientations was obtained from a region of the specimen. Figure 8 presents the results of an EBSP analysis obtained along the gauge length of a $<110>$ oriented specimen that was tested to failure at 850°C, 550MPa with a total strain to failure of 5.8%. It is important to note that the EBSP technique has a high spatial resolution (approximately 1μm) and is able to determine the orientation close to the fracture surface of the specimen at high levels of strain where X-ray measurements are not possible. The model predictions for rotation are summarised in Figure 9. On this representation, initial orientations near $<$001$>$ and $<$111$>$ rotate to $<$001$>$ and $<$111$>$ respectively. In contrast, orientations near $<$011$>$ are not stable and in general rotate away from this orientation, as shown by the example in Figure 8. The predicted rotations in Figure 9 are also consistent with cube slip dominating for orientations close to $<$111$>$ and octahedral slip dominating for other orientations.

Other factors must be considered when analysing the results of EBSP. For example, Figure 10 presents the results of an analysis for a specimen with an initial orientation close to $<$112$>$. Scatter in the measurements increases with distance along the gauge length approaching the deformation neck and fracture surface and these large rotations were associated with interdendritic porosity, such that presented in Figure 11. Orientations measured in the vicinity of the pores showed large deviations from the average.

![Figure 8: Stereographic triangle showing EBSP measurements for a $<110>$ specimen of SRR99 creep tested at 850°C, 550MPa. The direction of rotation is indicated by the arrowed line.](image8)

![Figure 9: Model predictions for crystallographic rotation of the tensile axis.](image9)

![Figure 10: Stereographic triangle showing EBSP measurements for a $<112>$ specimen of SRR99 taken from the threaded end, middle and fractured end (right to left) showing the increasing degree of scatter as the fracture surface is approached.](image10)

![Figure 11: Secondary electron image showing the matrix of points used to obtain the EBSP data.](image11)
Validation from High Temperature Mechanical Testing

If the model is to be used for other design purposes, it must be capable of representing generalised deformation under a wide range of loading conditions. Various types of high temperature mechanical behaviour have been examined and compared to model predictions. Here we compare the results of slow strain rate controlled tensile tests on specimens of various orientations with simulations from the model with parameters determined from creep tests.

Figure 12a shows the experimentally determined tensile curves for <011> oriented specimens tested at 950°C at various strain rates; the model simulations are shown in Figure 12b. Clearly the general shapes of the curves are correctly modelled; after yield the ultimate tensile strength is achieved at 1 to 2% strain and thereafter there is a steady decline in stress. This softening is a direct parallel to the extensive tertiary creep behaviour that is observed. The qualitative agreement is good at the lowest strain rate (10⁻⁷ s⁻¹), but the model over estimates the tensile strength at higher strain rates. Since the database from which the model parameters were derived had creep rates of less than or equal to 10⁻⁷ s⁻¹, the result indicates difficulties in extrapolating to different strain rates.

The effect of orientation on the tensile behaviour is shown in Figure 13 for tests at a strain rate of 10⁻⁷ s⁻¹ and 950°C. In fact, very little anisotropy is predicted, and the results for <001> and <110> specimens are accurately represented by the model. The stress for the <112> falls off much more rapidly than predicted.

Figure 13: Experimental and modelled stress-strain curves for three different orientations of specimen tested at 10⁻⁷ s⁻¹ at 950°C.

Conclusions

A model for anisotropic creep deformation has been applied to the single crystal superalloy SRR99. The model has been validated using both macroscopic measurements of specimen deformation such as changes in cross-sectional shape and crystallographic rotation and high temperature strain-rate controlled mechanical tests. Agreement between the model predictions and experimental data is good; however, microstructural features such as evolution of γ' morphology and interdentritic porosity may dominate the deformation of the materials and the model is currently being evaluated with respect to these features.
Acknowledgements

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References


Appendix: Constitutive equations for anisotropic creep in single crystal superalloys

The constitutive equations used in the present study are required to represent two important aspects of the creep deformation of single crystal superalloys: the anisotropic deformation characteristics associated with crystallographic orientation and the highly nonlinear variation of creep rate with either strain or time.

A crystallographic model has been adopted in which deformation is considered to occur by shear on a restricted number of slip systems, \( \{a, b, c\} \). In particular, for single crystal superalloys slip is only allowed here to be on the families of systems of the type \((111)(110)\) and \((001)(110)\). The rate of shear deformation \( \dot{\gamma} \) on any of the \( k \) allowed slip systems will be a function of the resolved shear stress in that direction and the total strain of the body can be computed by summing all possible shear displacements:

\[
\epsilon = \sum_{k=1}^{\infty} \dot{\gamma} n_k
\]

This leads to both a change in orientation of an arbitrary direction from \([x_1, x_2, x_3] \) to \([X_1, X_2, X_3] \):

\[
\begin{bmatrix}
X_1 \\
X_2 \\
X_3
\end{bmatrix} =
\begin{bmatrix}
1 + \epsilon_1 & \epsilon_{12} & \epsilon_{13} \\
\epsilon_{21} & 1 + \epsilon_{22} & \epsilon_{23} \\
\epsilon_{31} & \epsilon_{32} & 1 + \epsilon_{33}
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
\]

and a linear strain in that direction of \( \epsilon = X - x \). The shear strain rate \( \dot{\gamma}_k \) on each of the two families of slip systems is considered to depend on two state variables; an internal stress \( S \) that dominates at low strains leading to primary creep deformation and a damage parameter \( d \) that is most important at higher strains leading to tertiary creep deformation. The specific equation set used in the present study is:

\[
\dot{\gamma}_k = \gamma_k \left( 1 - \frac{S_k}{S'} \right) \left( 1 + \omega k \right)
\]

\[
\dot{S}_k = H_k \dot{\gamma}_k \left( 1 - \frac{S_k}{S'} \right)
\]

\[
\omega_k = \beta_k \dot{\gamma}_k
\]

The shear deformation on the particular slip system for a fixed temperature and shear stress is determined by the four constants \( (\gamma^k, H^k, S^k, \beta^k) \). This parameter set was determined for the octahedral shear system by analysis of some 35 constant stress tensile creep tests at a range of temperatures and stresses for \(<001>_1 \) orientations of SRR99. Cube shear parameters were determined from a smaller database creep curves for \(<111>_1 \) specimens.

Each of the model parameters, \( P = (\dot{\gamma}^k, H^k, S^k, \beta^k) \) are represented by exponential functions of shear stress \( \tau \) and temperature \( T \):

\[
P = a \exp \left( b \tau - \frac{Q}{RT} \right)
\]

The database examined is well represented by the values of the parameter listed in the Table.

<table>
<thead>
<tr>
<th>Parameter ( P )</th>
<th>( a ) (MPa(^{-1}))</th>
<th>( b ) (MPa(^{-1}))</th>
<th>( Q ) (J mol(^{-1}))</th>
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</thead>
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<td>Octahedral shear</td>
<td>( \dot{\gamma}^k )</td>
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<td>4.49x10(^{-2})</td>
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<tr>
<td>( H^k )</td>
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</tr>
<tr>
<td>( S^k )</td>
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<td>0</td>
</tr>
<tr>
<td>( \beta^k )</td>
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<td>-1.20x10(^{-2})</td>
<td>0</td>
</tr>
<tr>
<td>Cube shear</td>
<td>( \gamma^k )</td>
<td>1.94x10(^7)(s(^{-1}))</td>
<td>3.73x10(^{-2})</td>
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</tr>
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</tr>
<tr>
<td>( \beta^k )</td>
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