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Extension of an anisotropic creep model to general high temperature deformation of a single crystal superalloy

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Abstract

A physics based model has been developed that accounts for the principal features of anisotropic creep deformation of single crystal superalloys. The present paper extends this model to simulate other types of high temperature deformation under strain controlled test conditions, such as stress relaxation and tension tests at constant strain rate in single crystals subject to axial loading along an arbitrary crystal direction. The approach is applied to the SRR99 single crystal superalloy where a model parameter database is available, determined via analysis of a database of constant stress creep curves. A software package has been generated to simulate the deformation behaviour under complex stress-strain conditions taking into account anisotropic elasticity.

1. Introduction

In order to achieve the full potential of single crystal superalloys currently in use as turbine blades, it is necessary to obtain a comprehensive description of the anisotropy of their mechanical behaviour. Previous work by Ion et al [1] and Barbosa et al [2] showed the possibility of predicting high temperature mechanical properties of isotropic materials, in particular high temperature creep deformations, utilising physics-based models. This approach has been extended by Ghosh et al [3] to account for anisotropic creep in single crystals where deformation is restricted to a limited number of slip systems. The features that can currently be incorporated in the modelling of anisotropic creep deformation as part of the work carried out by the present authors, include (a) creep for single crystals at arbitrary crystallographic orientation, under either uniaxial tension, compression, or multiaxial stress state; (b) deformation along any crystal direction specified, such as strain in specimen cross section, and specimen shape change; and (c) crystal rotation during creep. McLean et al [4] have reported a preliminary validation of this type of anisotropic modelling, comparing the measured crystal rotation and specimen shape change in creep test with model predictions.

Predictive calculations have been made by Ghosh and McLean [5] through extending the constitutive equations for isotropic creep deformation to simulations of other more generalised high temperature deformations. The present work explores the anisotropic creep approach to the characterisation of anisotropic stress-strain relationships in single crystal alloys under more generalised test conditions. Supplemented by the elasticity data of the alloys, simulations of time dependent deformations in constant strain rate test, as well as stress relaxation of pre-loaded crystals, are made with computer software generated to perform the model calculations.

2. Model Formulation for Anisotropic Creep

In the isotropic model the creep strain rate is considered to be influenced by a variety of damage mechanisms. By defining a dimensionless damage parameter ω to represent tertiary creep behaviour and relating the state variable with the plastic strain, a description of creep curves is given by the following coupled set of differential equations:

$$\dot{\varepsilon} = \dot{\varepsilon}_i (1 + \omega)$$
$$\dot{\omega} = C\, \dot{\varepsilon} \qquad (1)$$

where ε is the tensile strain, $\dot{\varepsilon}_i$, and C are constants [6]. When the model parameters are defined, creep curves can be calculated by numerical integration of the differential equation set.

The tensile creep formulation given above has been successfully used in modelling isotropic mechanical behaviour. To extend the formulation to modelling single crystal anisotropic deformation, shear strains on each activate slip system are calculated using the same formulation for the differential equation set, expressed in terms of shear strain and the damage parameter ω:

$$\dot{\gamma}^k = \dot{\gamma}_i (1 + \omega)$$
$$\dot{\omega} = \beta\, \dot{\gamma}^k \qquad (2)$$

γ^k is the shear strain on the activate slip system where *k* denotes one of the activate slip systems, and $\dot{\gamma}_i$ and β are the model parameters [3]. The equivalent total strain along a given direction can be calculated by summing the contributions from all the operating slip systems.

It is necessary to describe the model parameters via appropriate functions of stress and temperature in order to interpolate and extrapolate from a limited database to various test conditions. According to the previous work of Curtis and McLean [7] the initial characteristic creep rate for the single crystal superalloy SRR99 is well represented by an exponential relation with stress and temperature:

$$\dot{\gamma}_i = A_1 \exp(A_2\, \tau^k - Q_1/RT) \qquad (3a)$$

where A_1, A_2 and Q_1 are the model constants, R is the gas constant, T is temperature, k again denotes one of the operating slip systems, and τ^k is the resolved shear stress on the *k*th slip system. The other model constant β can be written by adopting the formula used for the initial creep rate $\dot{\gamma}_i$:

$$\beta = A_3 \exp(A_4\, \tau^k - Q_2/RT) \qquad (3b)$$

where A_3, A_4 and Q_2 are constants. The model constants for single crystal SRR99 used in the present calculation are as given in Table 3 of Ghosh et al [6].

The contribution of shear on all the activate slip systems gives rise to strain or deformation gradient, usually denoted by a tensor, ε_{ij}, having six independent components. The suffixes i, j represent components along the three cubic crystal axes and have integer values of 1, 2 or 3 only. This strain tensor is anisotropic in general, and can be determined by the magnitude of shear strain γ^k and geometry of the slip systems:

$$\varepsilon_{ij} = \Sigma\, \gamma^k\, b_i^k\, n_j^k \qquad (4)$$

Here the *k*th slip system is defined by a unit vector, **n**, normal to the slip plane, and by a unit vector, **b**, in the slip direction. The summation is performed over all the possible slip systems. The anisotropy of creep deformation in a single crystal is therefore readily accounted for using the shear model formulation.

3. Simulation of Strain Controlled Tests

Though originally developed to treat creep curves under constant stress, the model formalism can be extended to simulations of high temperature deformations under other more generalised stress conditions. In the strain controlled tests considered here, the total strain (ε_{total}) along the specimen crystallographic orientation <hkl> is either kept at the pre-strain level, as in the stress relaxation test, or is increased with time, as in the constant strain rate test. The uniaxial stress along the <hkl> direction corresponds to, by Hooke's law, the Young's modulus along the <hkl> direction $E_{<hkl>}$:

$$\sigma = E_{<hkl>} (\varepsilon_{total} - \varepsilon_{creep}) \qquad (5)$$

In order to introduce this anisotropic modulus in the model calculation, it is necessary to incorporate a description of the full elastic behaviour of the alloy. The Young's modulus $E_{<hkl>}$ can be specified in terms of the compliances S_{ij} via the transformation rule for tensors. For a material with cubic symmetry, such as the single crystal superalloy under consideration, it is sufficient to specify the three none-zero elements of the compliance tensor [S]: S_{11}, S_{12}, S_{44} [8]. If h, k, l are the direction cosines of the [hkl] vector, ie, [hkl] is the unit vector,

$$1/E_{<hkl>} = S_{11} + \{S_{44} - 2(S_{11} - S_{12})\} (h^2k^2 + k^2l^2 + l^2h^2) \qquad (6)$$

The full compliance tensor for the single crystal superalloy SRR99 is derived from the measured data on $E_{<100>}$, $E_{<111>}$, and limited data on $G_{<100>}$ available for temperatures ranging from 20°C to 1200°C.

By adopting a time stepping sequence, the problem is to calculate the creep strain at each time interval. This can be done by resolving the tensile stress to the respective shear stress on each activate slip system and defining the model parameters by following the relations given in equation (3a) and (3b). The differential equation set (2) can then be integrated to obtain the shear strain on the possible slip systems for the Ni-based fcc single crystal, which include 12 cubic type {100}<011> and 6 octahedral type {111}<$\bar{1}$10>. The creep strain along the <hkl> direction can be derived via geometric factors, once the deformation gradient for the crystal is determined. As long as the initial strain conditions are defined, the results of the iteration will be dependent only on the step size. The calculation results will converge when the step size is infinitely small. It was found that a step size Δt of 0.1hr is good enough for the present work to bring the uncertainty in the calculated stress down to less than 0.2MPa, although the choice for an appropriate step size in other calculations should be confined by the time scale considered.

4. Simulation Results and Discussion

The algorithm described above is implemented in to the software package the present authors have previously generated for modelling anisotropic creep deformations. The routines are written in C programming language on a Sun Sparc workstation. Using the software it is possible to calculate the variation of stress in a stress relaxation process at a defined pre-strain level for a given crystal orientation. The software can also be used to calculate the stress-strain curve in a tensile test at a constant strain rate for a given crystal orientation. It should be pointed out that simulations can be made for any arbitrary crystal orientation, and at any temperature where elasticity data are available.

The stress-strain curves simulated for tension tests of the single crystal with <123> orientation at 850°C at strain rate of $1x10^{-5}$, $1x10^{-6}$, and $1x10^{-7}$ s^{-1}, are shown in Figure 1. All curves show a peak stress, followed by a progressive decrease in stress. Comparison between the stress-strain curves of tension tests at 850°C and a strain rate of $1x10^{-7}$ s^{-1} simulated for SRR99 single crystal <100>, <111>, and <211> orientations are shown in Figure 2. The initial slopes of the three stress-strain curves before the peak stresses are reached correspond to the Young's moduli of the alloy at the respective orientations, with $E_{<111>} > E_{<211>} > E_{<100>}$. However, there is

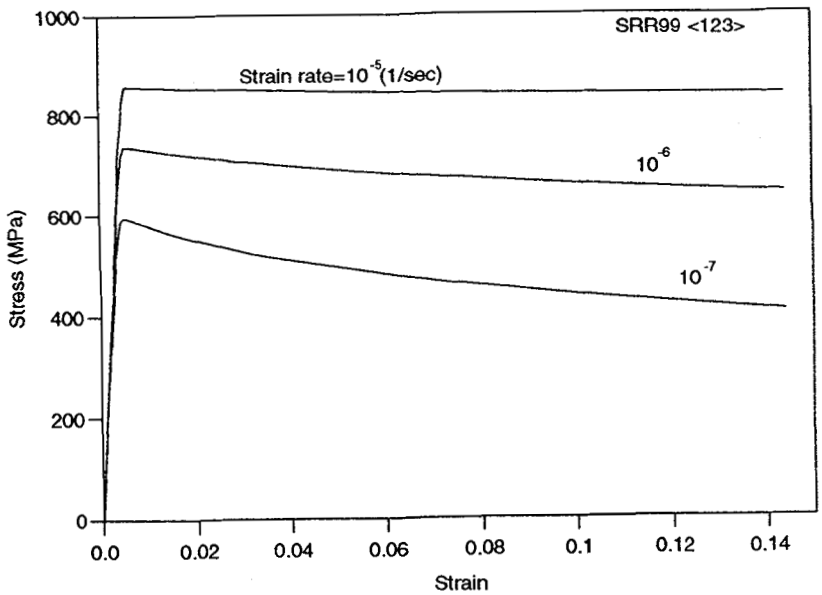

Figure 1. Simulated stress-strain curve at 850°C for the SRR99 single crystal of <123> orientation at different strain rate.

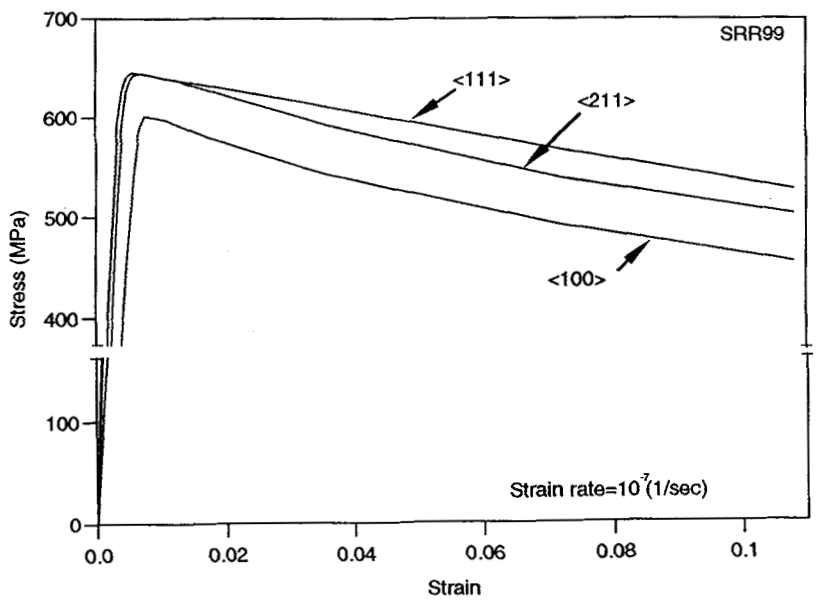

Figure 2. Comparison of the simulated stress-strain curves at 850°C for the SRR99 single crystal of <100>, <111>, and <211> orientations at a strain rate of 1×10^{-7} s^{-1}.

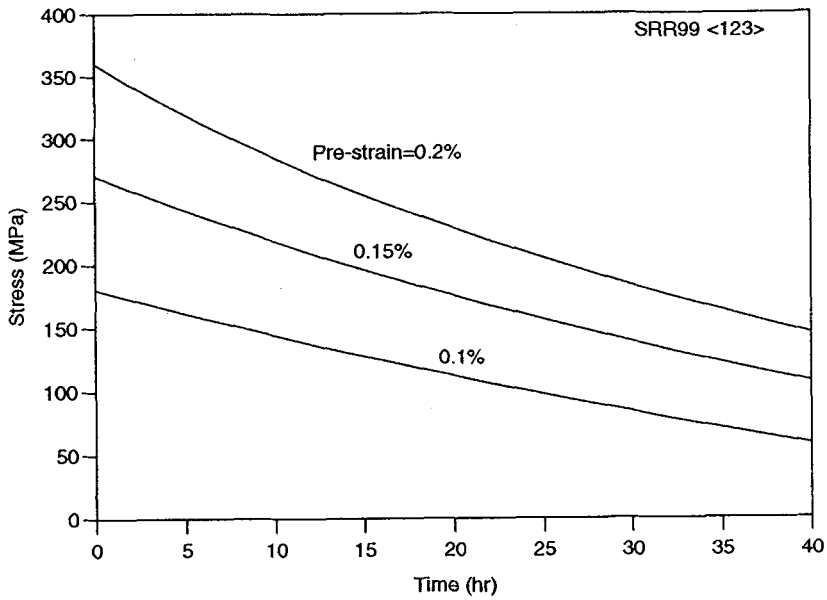

Figure 3. Simulated stress relaxation at 850°C for the SRR99 single crystal with <123> orientation at various level of pre-strain.

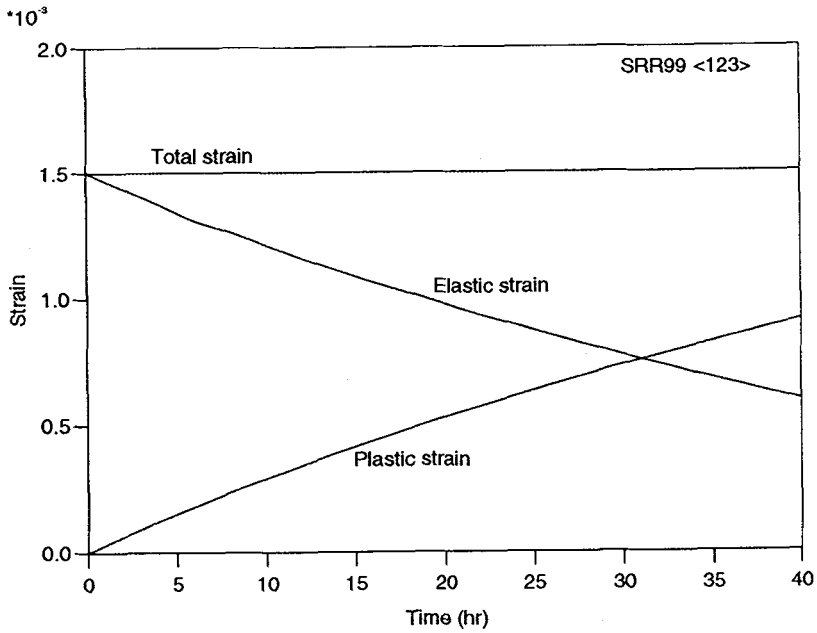

Figure 4. Strain distribution during stress relaxation (pre-strain 0.15%) at 850°C for the SRR99 single crystal of <123> orientation.

also a predicted difference in the ultimate stresses. Figure 3 shows the simulation results of stress relaxation for the SRR99 single crystal with <123> orientation at 850°C, with pre-strain at 0.2%, 0.15%, and 0.1%. The initial stress is determined using Hooke's law, assuming the pre-strain being completely elastic. The decrease in stress during the relaxation is accompanied by the introduction of creep (plastic) strain, as is shown in Figure 4, for a pre-strain of 1.5%. The plastic strain will be increasing with time, approaching the pre-strain level. The stress will eventually be completely relaxed with infinite time, when the elastic strain reaches zero.

It should be noted that plastic strain can be defined along not only the initial crystal orientation, but also any other directions. For example, strains along the directions in the cross section of the specimen can be calculated following this algorithm. The final shape of the cross section is expected to be elliptical, considering the model calculation as well as the experimental results for single crystal creep. The crystal orientation is also expected to rotate during the deformation, except in the few symmetrical directions, such as <100> and <111>, due to the anisotropy of the deformation for a crystal of an arbitrary orientation. In this case the simulation is only realistic if a stepping sequence is used, so that the deformation is accounted for by strain summation carried out along the changing orientation over each step. On the other hand, the actual stress state is not strictly uniaxial in a test specimen, especially at the ends fixed to a tensile machine, of a single crystal at an arbitrary orientation because of the crystal rotation effect. It remains to be seen as to whether the complexity introduced by the multiaxial stress state as the boundary condition in a strain controlled test can be readily reduced in the framework of 18 possible operating slip systems.

Now that the software interpolates and extrapolates mechanical behaviour of the single crystal alloy under various test conditions, it is necessary to carry out critical validation experiments to test the predictions made by the model calculations. With a full description of the anisotropic behaviour available for a single crystal alloy, it will be possible to utilise finite element method to analyse the performance of a component which subjects to a distribution of complex stress condition in application. The present model calculation serves as a basis for any subsequent finite element analyses by providing the data necessary for the properties of the material elements, in particular the anisotropic properties of the single crystal under arbitrary loading conditions.

5. Conclusions

The formalism for anisotropic creep deformation has been extended to simulate deformations in stress relaxation and tensile tests at high temperature for arbitrary crystal orientations of a single crystal. The stress-time or stress-strain curves have been calculated for stress relaxation and tension tests at constant strain rate for single crystal SRR99 following the simulation procedure, together with the knowledge of anisotropic elasticity of the material.

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