Continuum Damage Mechanics Modeling of Creep in DS GTD-111\textsuperscript{TM} Superalloy
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Abstract

Safe extrapolation of short-term creep data requires development of creep models where (a) the constitutive laws are physics based, and (b) majority of model parameters are calculated rather than empirically fitted. This paper details the structure of such a physics-based creep model and its application to DS GTD-111\textsuperscript{TM} superalloy. The constitutive creep law is derived from the kinetics of dislocation-particle interactions in the presence of thermal activation. This constitutive creep law is further coupled with the evolution kinetics of controlling microstructural parameters and associated damages. The model is expected to provide vital inputs for component design as well as remaining life assessment. (GTD-111\textsuperscript{TM} is a trademark of the General Electric Company).

Introduction

Creep refers to thermally assisted accumulation of plastic strain in a material, at stress levels usually below its yield strength. This accumulation of plastic strain in an engineering component can lead to unacceptable levels of dimensional changes, shape changes, and/or eventual rupture. Gas turbine hot gas path components have design strain limits, beyond which they are deemed to have failed.

Accordingly, it is critical to be able to predict the time taken for a component to accumulate this design strain at operating stress and temperature levels. Most existing design methodologies achieve this by generating a limited amount of short-term creep data and empirically fitting it to:

- a simple analytical/differential equation viz. power law or θ-projection, that relates the rate of accumulation of creep strain to the operating stress and temperature, or
- a time-temperature parameter viz. Larson-Miller or Orr-Sherby-Dorn parameters.

These empirical fits are then extrapolated to determine the combinations of stress, temperature and time (σ, T, t) that allow safe operation. However, these extrapolations do not account for the continual evolution of material microstructure that normally has a damaging effect on its creep strength. The risk is that these extrapolations to longer times lead to a non-conservative estimation of useful life, forcing designers to add large safety factors to the estimated operating life. While this exercise does have the desired effect of making the design fail-safe, it raises an important question: “are we retiring these expensive components too early, and missing out on useful life?”

The only way to address this paradoxical situation is to develop physics-based models of creep deformation that implicitly account for evolving microstructure and associated damages. In the present paper we report our efforts towards development of such a model, within the framework of Continuum Damage Mechanics (CDM) for DS GTD-111 nickel-based superalloy.
Material

DS GTD-111 is a directionally solidified high-performance nickel-based superalloy that is extensively used for industrial gas turbines buckets manufacturing. The nominal composition of this alloy is given below in Table 1, and it is heat-treated to give a two-phase \( \gamma-\gamma' \) microstructure. A typical example of its microstructure in standard heat-treated condition is given in Fig. 1. The \( L1_2 \) ordered \( \gamma' \) precipitates are present in a bi-modal distribution and their total volume fraction is approximately 55%.

**Table 1. Chemical composition of superalloy DS GTD-111.**

| Element | Ni | Cr | Co | Al | Ti | Mo | C  | W  | Ta |
|---------|----|----|----|----|----|----|----|----|----|
| [weight %] | 60.5 | 14 | 9.5 | 3.0 | 4.9 | 1.5 | 0.1 | 3.8 | 2.8 |

Fig. 1. DS GTD-111 typical microstructure in standard heat-treated condition.

Creep mechanism and quantitative model

Nickel-based superalloys are strengthened by the presence of coherent and ordered precipitates. These precipitates act as effective barriers to dislocation motion and the dislocations are forced to climb around them. Climb being a non-conservative process, requires flow of vacancies towards or away from the dislocation line, making the whole process diffusion controlled. The classic theory of Ansell and Weertmen [1] represented creep in particle-strengthened materials as sequential climb & glide and also derived simple quantitative expressions for strain rate. While this picture is still widely accepted, the strain rate equations have since been refined by many researchers, notably by Brown and Ham [2], who carried out detailed calculations for creep rates in particle-strengthened materials for the more realistic case of localized climb. Ion et al. [3] recognized that it is not sufficient to derive a physics based creep law; one also needs to account for the evolution of internal stresses in the material as well as that of the microstructure. This framework was referred to as Continuum Damage Mechanics (CDM) and has since been refined and applied to many material systems [4-6].
In the present study, which focuses on DS GTD-111 superalloy, we have used the following description of creep to construct a quantitative model:

- Creep strain accumulation is limited to the matrix phase, with limited or no dislocation activity in the precipitate.
- Dislocations overcome the precipitate by a diffusion-controlled climb process, and then they glide freely till they hit another precipitate.
- The glide process is instantaneous and infinitely faster compared to the climb time.
- The mismatch of plastic strain rates between the two phases leads to an effective stress-transfer from the precipitate to the matrix.
- The stress transfer rate is directly proportional to elastic modulus and overall creep strain rate.
- Below the yield stress of the material, the maximum possible stress transfer depends on the relative volume fraction of the two phases.
- This stress transfer lowers the effective stress in the matrix, leading to a continuously decreasing creep rate. When the stress transfer process is complete, the strain rate reaches a steady state.
- The strain rate would continue to remain constant, but for the evolution of the underlying microstructure viz. increase in mobile dislocation density and coarsening of the γ'.
- These microstructure changes lead to a continually increasing strain rate and eventual rupture.

Quantitative representation of these concepts leads us to the following set of constitutive equations:

\[
\dot{\varepsilon} = \dot{\varepsilon}_0 \frac{Q_{j/v}}{RT} \frac{1}{(1 - D_p)} \text{Sinh} \left( \frac{\sigma - \sigma_{in}}{\sigma_0(1 - D_p)} \right),
\]
(1)

\[
\dot{\sigma}_{in} = h' \left[ 1 - \frac{\sigma_{in}}{\sigma H^*} \right] |\dot{\varepsilon}|.
\]
(2)

\[
\dot{D}_d = C(1 - D_d)^2 |\dot{\varepsilon}|.
\]
(3)

\[
\dot{D}_p = \frac{k'}{3}(1 - D_p)^4.
\]
(4)

Eq. 1 is the constitutive creep law that has been derived based on the above framework, and its details can be found elsewhere [4-6]. \(\dot{\varepsilon}_0\) is a reference strain rate and depends on precipitate size, volume fraction and dislocation density. \(Q_{j/v}\) is the activation energy for self-diffusion, combined with that of dislocation jog formation. Formation of dislocation jogs is required for the climb process. \(\sigma_0\) is a reference stress that varies inversely with obstacle spacing. We then recognize the fact that there will be a stress-transfer from the matrix to the precipitate, and that creep process in the matrix will be governed by effective stress in the matrix \(\sigma - \sigma_{in}\), where \(\sigma_{in}\) is an evolving internal stress and its evolution is governed by Eq. 2.

\(D_p\) and \(D_d\) are normalized and dimensionless damage parameters associated with dislocation multiplication and particle coarsening, and are defined as:

\[
D_p = \left( 1 - \frac{\lambda_0}{\lambda} \right) \quad \text{and} \quad D_d = \left( 1 - \frac{\rho_0}{\rho} \right).
\]
(5)
$C$ and $k'$ are the rate constants associated with dislocation multiplication and particle coarsening, while $\lambda$ and $\rho$ represent respectively the interparticle-spacing and dislocation-density parameters ($\lambda_0$ and $\rho_0$ are their starting values). The damages defined above evolve from 0 in the initial undamaged-reference-state and approach 1 when $\lambda$ and/or $\rho$ become increasingly larger. These equations, when solved simultaneously, describe the evolution of creep strain as well as associated microstructural damages at any given stress and temperature. Most of the model parameters are related to the underlying microstructure and are known within reasonable bounds. Some parameters, viz. rate constants for precipitate coarsening, can be assessed from independent thermal aging experiments, while the remaining few parameters viz. $\dot{\varepsilon}_0$ and $C$ are calibrated using a limited amount of experimental creep data.

**Results and Discussions**

A limited number of creep tests were carried out in the temperature range of 800-950°C and at stress levels in excess of the in-service ones. Some of these tests were interrupted at strain levels in the range 0.2–2.0% strain to identify the deformation mechanisms and to validate the above mentioned assumptions, while others were run till rupture. Example TEM micrographs of deformed specimens after 1% creep strain are presented in Fig. 2 (in this and in the following figures $T_1<T_2<T_3$ and $\sigma_1<\sigma_2<\sigma_3$). Across the stress-temperature regimes of interest, the dislocation activity is found to be limited to the matrix phase and we do not observe any particle cutting at the relatively high stress levels investigated. Fig. 2 also shows the presence of dislocations held up at the matrix-precipitate interface, and these act as agents of stress transfer between the two phases. These observations are in line with our view of creep deformation in this material.

![Fig. 2. Typical deformed microstructures after 1% creep strain at different stress and temperature conditions. Most of the dislocation activity is limited to matrix phase.](image)

As mentioned earlier, one can arrive at reasonable estimates of most of the model parameters if one has quantitative information on:

- Average starting size of the $\gamma'$ precipitate;
- Their volume fractions as a function of temperature;
- Their rate of coarsening;
- Elastic modulus of the alloy at the temperature of interest;
- Estimates of vacancy diffusivity in the matrix phase.
A combination of thermo-kinetics calculations viz. ThermoCalc™, quantitative image analysis on SEM images, and experimental data on elastic moduli were used to arrive at these initial estimates. The optimal values of the complete parameter set were then found by carrying out a constrained optimization against a limited amount of creep data.

The constitutive equation set, (Eqs. 1-4), is able to capture not only the time-to-reach-a-given-strain but also the complete creep curve. These comparisons, over a range of stress and temperature conditions, are presented in Figs. 3-4 respectively.

**Fig. 3.** Comparison of experimental data and model predictions for time to reach 1% creep strain over a range of stress and temperature.

**Fig. 4.** Comparison of experimental data and model predictions for the complete creep curves over the investigated range of temperature.
Application of the model to a different starting microstructure would require scaling the microstructure-dependent parameters appropriately. For example, if one starts with a coarser microstructure the starting value of $\sigma_0$ will be correspondingly lower. A service-exposed material that has a coarser microstructure as well as a higher dislocation density, will not only have a lower value of $\sigma_0$ but also a correspondingly higher value of $\dot{\varepsilon}_0$. The modulus and the precipitate volume fraction decrease with increasing temperature and this will be reflected in the temperature dependence of the stress-transfer parameters. As stated earlier, the coarsening kinetics rate constant $k'$ is obtained from independent set of experiments and the diffusivity is also known within reasonable bounds from independent sources.

It will be important to mention at this point that although this particular alloy has a bi-modal distribution of the strengthening precipitate, we have considered:

- Total precipitate volume fraction for the purpose of determining the extent of stress transfer;
- Inter-particle spacing of the larger population for the purpose of determining $\sigma_0$.

**Summary**

In the present study, we have developed a quantitative model of creep deformation in DS GTD-111 that has the following key features and assumptions:

- The model views accumulation of creep strain to arise from a localized climb & glide process.
- The model implicitly accounts for changes in material microstructure and associated damages.
- The model uses a single creep rate equation to capture the whole creep curve. This is in strong contrast with some existing approaches, which treat different stages of a creep curve to arise out of independent processes and linearly add their contributions.
- The model has very few number of total model parameters. Additionally most model parameters have explicit relationship to measurable material properties and its microstructure, and this makes the model applicable to different starting microstructures with relative ease.
- Finally, if one uses the microstructure of service-exposed material to compute the model parameters, one can in principle predict the remaining life of the hardware.

Further work is required to test the model against a range of different starting microstructures as well as service-exposed hardware.

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