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Modelling of thermomechanical fatigue stress relaxation in a single-crystal nickel-base superalloy

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ABSTRACT

The thermomechanical fatigue (TMF) stress relaxation of the single-crystal nickel-base superalloy MD2 has been analysed and modelled in this paper. In-phase and out-of-phase TMF experiments in the nominal [0 0 1], [0 1 1] and [1 1 1] crystal orientations have been performed. The TMF cycle consists of two loadings each with a 100 h long hold-time. A simple crystallographic creep model, based on Norton's creep law, has been developed and used in conjunction with a crystal plasticity model. The model takes anisotropy and tension/compression asymmetry into account, where the anisotropic behaviour is based on the crystallographic stress state. The values of the creep parameters in the anisotropic expression were determined by inverse modelling of the conducted TMF experiments, a parameter optimisation were performed. The developed model predicts the stress relaxation seen in the TMF experiments with good correlation.

1. Introduction

The market for renewable energy technologies is continuing to grow, and an increase of renewable sources like wind and solar power is expected. Since the production by such sources cannot be actively planned, the grid must be built in such a way that the wind or solar energy can be efficiently received when there is such production, but also so that one can manage over periods where there is none. In short, this means that the wind and solar energy power must be balanced by other power sources that can be regulated (up and down) on a minute-by-minute basis. This can, for instance, be achieved by gas turbines [1], and an increasing demand for gas turbines designed to stand high numbers of starts and stops can therefore be foreseen. The components in the hot sections of the gas turbine will experience thermomechanical fatigue (TMF) loading, *i.e.*, both thermal and mechanical cycling. Further, during the steady-state condition, also known as hold-time, under service load the components will undergo creep deformation if the temperature is sufficiently high, and the stress state will relax.

The hottest components in a power generating gas turbine are the blades and guide vanes of the first turbine stage. These are mainly produced in the state-of-the-art material, preferable single-crystal nickel-base superalloys which have excellent mechanical properties in very hot environments [2]. These materials will increase the efficiency of the gas turbine as a higher operating temperature can be achieved compared to other materials, which in turn reduces the fuel consumption, leading to reduced environmental effects and lower operating costs [3].

Single-crystal nickel-base superalloys have a face-centered-cubic crystal structure [4], with well defined crystallographic slip planes and slip directions. The material exhibit a well known elastic anisotropy and anomalous plastic behaviour, such as plastic anisotropy and tension/compression asymmetry, which are dependent on the crystallographic structure of the material. As the component is loaded, plastic flow will eventually occur, and the deformation will take place along the crystallographic slip planes, also known as crystal plasticity, see *e.g.* Haupt [5] or Roters et al. [6].

There are two main types of TMF cycles which can affect the components of the gas turbine, the in-phase (IP) TMF cycle and the out-of-phase (OP) TMF cycle. In the IP case the temperature is cycled in-phase with the applied mechanical strain, and in the OP case the temperature is cycled in reverse to the mechanical strain. The typical differences between the two types can be seen in Han et al. [7], where the deformation and damage mechanisms of the first generation single-crystal superalloy SRR99 was investigated for both IP and OP conditions. A display of the two different load cycles and the corresponding hysteresis loops, where one can observe the unsymmetrical shape of the stress–strain curve, can be found. The OP TMF behaviour with hold-time of the single-crystal

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superalloy CMSX-4 was investigated in Moverare et al. [8], where a practical TMF procedure is described. It is stated that the OP case is typically the one for the hottest region of a component, where a local point might experience compression at the peak temperature, a so called *hot-spot*.

At comparative low temperatures, at least in the case of gas turbines, 100–500 °C, a single-crystal superalloy is not likely to undergo creep deformation. As the components experience a TMF cycle, in which room temperature conditions might be reached, it is thus crucial that the low temperature constitutive behaviour of the material is correctly captured. In the work of Qin and Bassani [9,10] a physically inspired room temperature crystal plasticity model was developed using Schmid and non-Schmid stresses to take the observed anomalous plastic behaviour into account. The model manages to calculate the relative size of the tension/compression asymmetry in the $[0\,0\,1]$, $[0\,1\,1]$ and $[\bar{1}\,1\,1]$ crystallographic directions. This model was later enhanced by Leidermark et al. [11] to incorporate further non-Schmid stresses to be able to describe the low temperature behaviour of a single-crystal nickel-base superalloy. A comparison with experimentally made tension and compression tests of the single-crystal nickel-base superalloy MD2 were made with good agreement.

At higher temperatures, in the area of approximately 600–800 °C, the single-crystal material will start to experience time dependent deformation, creep, and in combination with the long hold-times at the steady-state condition resulting in relaxation of the stress state. There are many different types of creep models for single-crystal nickel-base superalloys, Ma et al. [12] proposed a microscopic dislocation model using dislocation glide and climb to account for the creep deformation of the single-crystal superalloy CMSX-4. Another dislocation model is presented in Zhu et al. [13], which couples the alloy chemistry to the creep deformation. A macroscopic viscoplastic model using the Orowan's assumption, that creep strain rate is proportional to the density of the mobile dislocations, has been combined with a rate-independent crystal plasticity approach by Staroselsky and Cassenti [14] to accommodate for the material behaviour of the single-crystal nickel-base superalloy PWA1484 in both LCF and OP TMF tests. In the paper of Ghosh et al. [15] an anisotropic dislocation creep model is described, which includes octahedral and cube slip in combination with a damage parameter that is dependent on the dislocation density. The model is able to predict the anisotropic creep response for a limiting set of experimental data. A phenomenological microscopic–macroscopic model based on rate-dependent crystal plasticity using a damage parameter following Kachanov's creep damage evolution for each slip system has been considered in the work of Vladimirov et al. [16]. The derived model was fit to uniaxial test data and validated for a multiaxial test case where a good agreement with primary, secondary and tertiary creep was obtained. Instead of incorporating the damage on the crystallographic level MacLachlan et al. [17] introduced a global damage tensor derived from the strain rate tensor to describe the creep deformation.

For even higher temperatures, 800–1100 °C, the material is also likely to undergo microstructural changes, so called rafting. Rafting is a time dependent process, that requires some induced plasticity, which gradually degrade the γ/γ'-microstructure and affects the mechanical properties of the material, for more details see *e.g.* Epishin et al. [18] and/or Leidermark et al. [19].

The objective of this paper is to model the TMF stress relaxation behaviour, creep deformation, observed in the single-crystal nickel-base superalloy MD2. Experiments have been made, where the three crystallographic orientations $[0\,0\,1]$, $[0\,1\,1]$ and $[1\,1\,1]$ have been investigated both in IP and OP TMF. Two TMF cycles each with a hold-time of 100 h have been applied, from which the creep response of the material is obtained. A new simplistic creep model is developed based on the creep deformation along the crystallographic slip planes. The model uses an anisotropic expression following the basic Norton creep law to define the amount of creep flow in each slip system. The TMF stress relaxation response from the experiments is used in an inverse modelling process (parameter optimisation) in which the creep parameters are determined through curve-mapping with the response from the FE-simulations. From the seen results of the parameter optimisation a good response is obtained, able to describe the anisotropic behaviour of the superalloy.

2. Experiment

The chemical composition of the investigated single-crystal nickel-base superalloy MD2 is Ni, 5.1Co, 6.0Ta, 8.0Cr, 8.1W, 5.0Al, 1.3Ti, 2.1Mo, 0.1Hf, 0.1Si (in wt.%). The material was solution heat treated at 1275 °C for 8 h followed by a two stage ageing process for 3 h at 1100 °C and 24 h at 850 °C. Six smooth test specimens were machined from cast bars with their longitudinal axes nominally parallel to the $[0\,0\,1]$, $[0\,1\,1]$ and $[1\,1\,1]$ crystal directions, two in each direction. The diameter of the specimens is approximately 6 mm and the parallel length is 24.58 mm, for more details regarding the geometry of the specimen please see Fig. 1. During the casting process a perfect aligned bar is almost impossible to achieve, thus all cast bars have a small misalignment in crystal orientation. The misalignment from the ideal longitudinal (primary) crystal orientations, denoted θ, varied between 1.8° and 6.2° for the specimens. The deviation from the ideal secondary crystal orientation (SCO), denoted ϕ, is of less concern than the primary deviation as the specimens are smooth and round. The nominal secondary crystal orientation can be either the $[1\,0\,0]$, $[\bar{1}\,0\,0]$, $[0\,1\,0]$ or $[0\,\bar{1}\,0]$ direction, for the nominal primary crystal orientation $[0\,0\,1]$. The misalignments and the individual diameters are listed in Table Table 1 for each specimen and the misalignments are defined according to Fig. 2. It is to be pointed out that θ and ϕ are defined with respect to the nominal $[0\,0\,1]$ crystal orientation regardless of primary orientation in the respective test specimens.

The specimens were alternately subjected to either an IP or an OP TMF cycle, *i.e.* $R_\varepsilon = \varepsilon_{min}/\varepsilon_{max}$ is equal to 0 and $-\infty$ respectively, where the temperature ranged between 100 °C and 750 °C in the loading. The mechanical strain range ($\Delta\varepsilon_{mech}$) of 1%, 0.7% and 0.6% were applied for the $[0\,0\,1]$, $[0\,1\,1]$ and $[1\,1\,1]$ crystal orientations, respectively. The difference in applied mechanical strain range is due to the fact that an initial equivalent inelastic strain (~0.5%) is to be present in the specimens for the different crystal orientations at the start of the hold-time. The TMF loading cycle was done in the following sequence: loading from 100 °C to 750 °C at a loading rate of 5 °C/s, a hold-time of 100 h was applied followed by an unloading with the reversed properties as in the loading stage, this sequence was then applied one more time to achieve two TMF cycles, see Fig. 3 for a more detailed overview.

The experimental TMF tests were performed in an Instron servo-hydraulic TMF machine using induction heating and forced air-cooling for rapid temperature changes. The testing machine was carefully aligned to prevent buckling of the specimens. A high-temperature extensometer with a gauge length of 12.5 mm was used during the tests, and in order to obtain the mechanical strain, the induced thermal strain was subtracted from the total strain. For a more detailed description of the experimental procedure see Segersäll et al. [20].

The reasons why only six test specimens were used in the study were due to the high manufacturing cost and availability of the single-crystal specimens, and consequently the statistical uncertainties in the analysis are bound to increase.