Modeling of cyclic stress-strain behavior and life prediction of near-α titanium alloy IMI 834 under thermomechanical fatigue conditions

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1 Introduction

The improvements in performance of jet engines has caused an increasing demand on the materials employed. In particular, the continuous increase in maximum operating temperature has resulted in loading conditions not accounted for in earlier life prediction models. A case in point are high-temperature titanium alloys used in the compressor part of jet engines. Initially design criteria focussed mainly on tensile and creep properties of the materials employed, and earlier titanium alloys such as Ti-6Al-4V had a rather modest maximum use temperature of about 315°C. By contrast, recent near-α alloys were designed with a target operating temperature of 600°C, and thus, much research has addressed high-temperature fatigue properties, oxidation and creep-fatigue interaction of such alloys, for a review see reference [1]. In actual high-temperature components, loading conditions are quite complex as these involve the combination of thermal transients with mechanical strain cycles during start-up and shut-down of the engine. It appears that the resulting thermomechanical fatigue (TMF) damage is already life-limiting in certain cases. As TMF was of no concern for earlier alloys, however, few studies have addressed this topic. Data obtained by Dai et al. [2] on Ti-6Al-2Sn-4Zr-6Mo has indicated that oxidation-induced embrittlement is a key issue in the TMF behavior of high-temperature titanium alloys. This study, however, was limited to 480°C. In the present paper results from research is reported that aimed at developing a life model for high-temperature titanium alloys that allows for extrapolation to service conditions of actual components.

2 Experimental Details

Near-α titanium alloy IMI 834 (nominal composition Ti-5.8Al-4.0Sn-3.5Zr-0.7Nb-0.5Mo-0.35Si-0.06C, in wt pct) was employed in the present study. The material was solution heat treated in the α/β phase at 1293 K for two hours in vacuum and oil quenched to obtain a bimodal microstructure consisting of primary α grains embedded in a lamellar transformed-β matrix. Metallography showed a volume fraction of about 18 pct equiaxed primary α grains with an average grain size of 14 μm. The material was aged at 700°C for two hours and air cooled in order to improve the mechanical properties through precipitation of fine silicides and ordered Ti3Al.

For fatigue testing, smooth cylindrical specimens with a gage diameter of 8 mm and a gage length of 14 mm were machined. In order to minimize surface effects on fatigue life, the samples were electropolished, and a surface layer of about 0.1 mm was removed in the gage section. All low-cycle fatigue (LCF) tests reported here were conducted under closed-loop fully reversed true plastic strain control using a triangular wave shape for the command signal.

The isothermal LCF tests were conducted over a temperature range from 350°C to 650°C. In the thermomechanical fatigue tests, the maximum temperature either coincided with the maximum plastic strain (in-phase TMF) or with the minimum plastic strain (out-of-phase TMF). Irrespective of the actual type of fatigue test, plastic strain rate in all fatigue tests reported here was 4 x 10^-5 s^-1. Further details on the LCF and TMF tests analyzed in the present study are given in reference [3].

3 Results and Discussion

3.1 Microstructure

As revealed by transmission electron microscopy (TEM), planar dislocation slip dominated deformation behavior in all isothermal fatigue tests conducted at test temperatures up to 600°C [3]. Similar to the isothermal LCF tests, planar dislocation slip within the primary α grains was observed in all TMF test as long as the maximum temperature of the TMF cycle did not exceed 600°C, cf. Figure 1. It is well established that the difference in critical resolved shear stress (CRSS) between the various slip systems favors a planar dislocation
slip mode in titanium alloys [4]. This effect is promoted further by the formation of shearable Ti$_3$Al precipitates during aging. Moreover, as a result of alloy partitioning effect aluminum is enriched in the primary $\alpha$ grains during solution annealing [5]. Thus, shearable Ti$_3$Al precipitates are formed predominantly within the primary $\alpha$ grains, and planar slip is most pronounced there. As a result of the strain localization within planar slip bands, fatigue cracks initiate preferentially within the primary $\alpha$ grains, cf. Figure 2.

If the test temperature exceeds 600°C, the differences in CRSS are diminished and cross-slip of dislocations starts to dominate deformation behavior. Hence, crack initiation no longer occurs at planar slip bands. Instead crack formation was observed to occur mainly within the lamellar transformed-$\beta$ matrix. Moreover, during extended high-temperature exposure an oxygen-enriched subsurface layer is known to form on titanium alloys. As fatigue cracks will form rather easily in this brittle layer, crack formation will be governed by the thickness of the oxygen-embrittled zone in case of long-term high-temperature tests, and microstructural effects on crack nucleation become negligible.

By contrast, stress-strain response in long-term high-temperature tests is significantly affected by microstructural instability. As shown recently [6], degradation of the lamella boundaries, which is promoted both by high-temperature exposure and plastic deformation causes a significant loss of cyclic strength, and stress-strain response of bimodal material gradually approaches that of equiaxed material.

3.2 Stress-Strain Model

In the present study a multi-component composite model [7, 8] was employed to predict stress-strain response of the material. In this model a material is considered as consisting of elements with different yield stress that are strained in parallel [9, 10]. This approach accounts for the microstructural heterogeneity observed in most materials. With respect to isothermal cycling the composite model has the striking advantage that all the parameters of the model can be obtained directly from a single branch of a stabilized stress-strain hysteresis loop. In TMF tests, the temperature changes continuously throughout the cycle. Thus, the temperature dependent yield stresses of the individual elements change cyclically as well. The TEM observations revealed that the microstructure established in TMF tests with a maximum temperature not exceeding 600°C is clearly dominated by planar dislocation slip, cf. Figure 1. In other words, similar microstructures prevail for isothermal fatigue tests and TMF tests in that temperature range. Hence, it is justified to assume that the stress-strain response at any given temperature within a TMF cycle can be calculated based on the isothermal material behavior at that specific temperature. Similarly, the stress-strain response in TMF tests with a maximum test temperature of 650°C, which is governed by a more wavy dislocation slip mode throughout the cycle, can be assessed based on isothermal tests run in the temperature regime where wavy dislocation slip prevails [3].

In Figure 3 an experimentally obtained hysteresis loop from a TMF test is compared to the model prediction. The predicted loop is based solely on isothermal tests, i.e. no additional fit parameters were involved. Note that Figure 3 shows data obtained on equiaxed material. As outlined above, this accounts for the fact that the bimodal microstructure displays pronounced microstructural instability in long-term high-temperature tests.

3.1 Life Model

*Isothermal Loading Conditions* - Both for isothermal LCF tests and TMF tests, large plastic strain amplitudes prevail, and thus, cracks nucleate early in fatigue life. In the present study is was assumed that fatigue life is governed completely by crack propagation. Hence, a microcrack propagation model was employed for life prediction. Such an approach is attractive from a physical point of view as fatigue damage is clearly defined by crack length.

The cyclic $J$-integral was proposed by Dowling [11] to correlate fatigue crack growth, if crack extension is driven purely by cyclic plasticity. The fatigue crack growth rate is then given by

$$\frac{da}{dN}_{fatigue} = C \times (Z_D)^m \times a^m$$  \hspace{1cm} (1)

where $C$ and $m$ are crack propagation constants determined from long crack growth behavior, and $a$ is the crack length. The damage parameter $Z_D$ was evaluated from the stress-strain hysteresis loop as suggested by Heitmann *et al.* [12]. The fatigue life is obtained by integrating Equation 1 between the initial crack length $a_0$ and the crack length at failure $a_f$. Life prediction is not very sensitive to the value assumed for $a_0$, and $a_f = 1$ mm was always used. By contrast, life predicted varies drastically with initial crack length. Extensive scanning electron microscopy (SEM) studies [13] have demonstrated, however, that initial crack length equals the size of the primary $\alpha$-grains for test temperatures where planar dislocation slip dominates. Similarly, initial crack length correlates with the size of lamellar transformed-$\beta$ grains under test conditions where wavy dislocation slip is the governing deformation mode.
Environmental effects are known to have a substantial effect on fatigue life of titanium alloys. At high temperatures, titanium alloys form non-protective oxide scales. Thus, oxygen diffuses rapidly into the metal matrix, and a brittle oxygen-enriched subsurface layers (α-case) forms. Microhardness measurements can be used to quantify the depth of oxygen-embrittled zone, as the hardness of the α-case layer has a square root dependency on oxygen concentration [14]. As seen in Figure 4, the microhardness in the α-case layer is increased significantly in a fatigued sample as compared to one that has been thermally exposed only. An enhanced uptake of oxygen by cyclic plastic straining has been reported for other materials as well [15, 16]. In the present study it was assumed that the different contributions to fatigue damage can be superimposed in a linear manner, i.e.

\[
\frac{da}{dN}_{\text{total}} = \frac{da}{dN}_{\text{fatigue}} + \frac{da}{dN}_{\text{oxidation}}
\]  

Reuchet and Rémy [15] suggested a model to calculate \(\frac{da}{dN}_{\text{oxidation}}\) for nickel-base superalloys. In the present study this model was adapted for titanium alloys, for details see reference 13.

Oxygen uptake becomes negligible at temperatures below about 500°C. Still, drastic environmental effects on fatigue crack growth do exist at even lower temperatures in titanium alloys, which can attributed to hydrogen-assisted crack propagation [17]. Again, these effects were modeled assuming that a linear superposition holds, and the environmental effect was assessed based on fatigue crack growth data obtained on IMI 834 in different environments and at different test frequencies [18, 19]. For details on the implementation of the model see reference 13.

**Thermomechanical Loading Conditions** – The term pure fatigue implies that damage evolves independent of time and temperature independent of the actual test mode. If this concept holds, TMF fatigue life in inert environments can be predicted using the cyclic \(J\)-integral approach in a straightforward manner. All that is needed is a modeled hysteresis loop such as the one shown in Figure 3. From this the elastic and plastic deformation strain energy densities are evaluated and the damage parameter \(Z_D\) of Equation 1 is calculated as suggested by Heitmann et al. [12] for isothermal tests.

In the present study the environmental contributions to fatigue damage under TMF loading were modeled mainly based on SEM observations. For instance, initial crack size in a TMF tests was found to be dependent on maximum temperature test experiment. Fractography indicated that in the case of in-phase TMF tests oxidation was the dominating environmental contribution to overall fatigue damage. By contrast, both hydrogen effects and oxygen-enhanced fatigue crack growth contributed to fatigue in the case of out-of-phase tests. Hence, out-of-phase testing is the most detrimental loading mode. Details on how these observations were implemented in the life model are given in reference 13.

Figure 5 shows a comparison between model predictions and experimentally obtained life data for isothermal LCF tests and TMF tests, respectively. All tests are predicted well within a scatter band of ± 2. More important, however, is to discuss the predictive capabilities if the model is to be applied to loading conditions significantly different from those used to establish the model. A case in point is cyclic stress-strain response. Given the instability of the bimodal microstructure, stress-strain data obtained on lower strength but cyclically very stable equiaxed material, cf. Figure 3, can be more appropriate if long-term behavior of the material is to be predicted.

Crack nucleation mechanism is the second key issue as the model employed relies heavily on accurate knowledge of initial crack length. It is known that crack nucleation mechanisms can differ significantly under isothermal and thermomechanical loading conditions, respectively [20]. IMI 834 is different in this respect as the dislocation slip mode governs the nucleation mechanisms in all short-term laboratory tests irrespective of the actual test mode. Thus, phenomena such as the change of crack density with mean stress observed in IMI 834 [6, 13] or the temperature dependence of the initial crack length are predictable based upon microstructural observations. In case of long-term high-temperature loading conditions, i.e. small plastic strain amplitudes, the formation of the α-case layer will govern crack nucleation. For small plastic strain amplitudes, however, plasticity-enhanced uptake of oxygen becomes negligible and the thickness of the α-case layer is easily predicted based on diffusion data.

Finally, the issue of coupling between the different damage mechanisms needs to be addressed. In the present study no coupling other than between plasticity and oxidation was allowed for. High-temperature titanium alloys appear to be quite different from most other materials in that oxygen-enhanced fatigue crack growth is governed by diffusion of oxygen into the bulk material, which should be unaffected by the presence of hydrogen. Similarly, the reaction of water vapor with freshly exposed material ahead of a propagating fatigue crack in the low-temperature part of a TMF loop should hardly be affected by prior oxidation in the high-temperature part of the cycle.

**4 Summary**
Isothermal and thermomechanical fatigue experiments were performed on near-α titanium alloy IMI 834 in order to develop a fatigue life model. The main results of this study may be summarized as follows:

1. A microcrack propagation model was applied successfully to predict fatigue life both under isothermal and thermomechanical fatigue conditions.
2. Planar dislocation slip governs both cyclic stress-strain response and crack nucleation in all fatigue tests conducted at temperatures not exceeding 600°C. If the temperature is increased significantly beyond 600°C, the dislocation slip mode becomes more wavy, and fatigue behavior changes accordingly.
3. For high-temperature fatigue tests, oxidation is the dominating environmental degradation mechanism. A strong coupling between plasticity and oxidation does exist. All other damage mechanisms are essentially uncoupled.
4. At test temperatures below about 500°C oxidation becomes negligible, and hydrogen embrittlement appears to be the main environmental effect.
5. Microstructural arguments can be used to assess the predictive capabilities of the model, and such observations are indispensable if the model is to be applied to loading conditions other than those used to establish the model parameters.

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