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Wavelet transformation based multi-time scale crystal plasticity FEM for cyclic deformation in titanium alloys under dwell load

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ABSTRACT

Titanium alloys are used in high end applications due to their desirable properties. However under dwell fatigue loading, these alloys exhibit premature crack initiation and failure when compared to normal cyclic loading. This early crack initiation can be attributed to the inhomogenous plastic deformation occurring in these alloys during the hold period of dwell cyclic loading and is strongly influenced by the underlying micro-structure. This necessitates the consideration of micro-structural features and their influence on the response, for accurate life prediction in these alloys. Crystal plasticity based finite element simulations capture the micro-structural influence on the response and can prove effective for accurate prediction of crack initiation in these alloys. However 70–80% of total life in Ti-alloys based components is spent in crack initiation and this may involve crystal plasticity based finite element simulations for large number of cycles. Such simulations using conventional single scale time integration schemes can be computationally intractable. A multi-time scale method using wavelet based decomposition is thus developed in this work for accurate and computationally efficient dwell fatigue simulations of these alloys for large number of cycles.

1. Introduction

Titanium alloys are used in high performance applications due to their high specific strength, toughness and corrosion resistance at elevated temperatures. However these alloys exhibit premature failure under dwell cyclic loading when compared to normal cyclic loading [1]. The early failure is strongly influenced by the underlying micro-structure and the micro-structural influence on the response should be considered when dwell fatigue life analysis of these alloys are performed. The conventional lifing techniques, like the total life approaches or the damage or defect tolerance approaches [2], are macroscopic in nature and the micro-structural effects on fatigue life are captured empirically by shifts in data curves after extensive testing. In total life approaches, like the stress-life or the strain-life approach, the number of cycles to failure is determined from stress amplitude of loading (S–N curves) or from the accumulated plastic strain (Coffin–Manson rule) [3] respectively. In damage or defect tolerance approaches, fatigue life estimates are based on propagation of a pre-existing crack from an initial size to final failure. Models such as the Paris law [4] are employed together with fracture toughness or threshold stress intensity factors to determine the number of cycles to failure. Although these methods work well under specific testing conditions, they exhibit significant scatter in their predictions. When these lifing techniques are used to design Ti-alloys based components, a great number of them retires prematurely even before damage initiation, thus shortening their full useful life.

The micro-structure of Ti-alloys are strongly anisotropic which causes inhomogenous plastic flow and strain localization to happen, during the additional hold period at the maximum applied stress in dwell cyclic loading. This necessitates the consideration of micro-structural features and its influence on response variations for accurate life predictions in these alloys. The important micro-structural features that affect the dwell fatigue behavior in Ti-alloys are grain orientations, misorientations, size, shape and grain boundary defects. Crystal plasticity based material models are effective in capturing the micro-structural influence on response [5]. Ghosh and co-workers [6–10] have extended the crystal plasticity theories to model deformation and creep mechanisms in Ti-alloys (Ti-6Al, Ti-6242). The model considers the grain orientation and misorientation distributions, the grain size distributions and morphology, and has been used in this work. Crystal plasticity based finite element simulations of representative micro-structure of Ti-alloys under creep conditions show stress concentration at grain boundaries [9]. This stress concentration is the driving factor that causes premature crack initiation in Ti-alloys under dwell cycle loading [11].

Fatigue failure in polycrystalline alloys starts with crack nucleation followed by steady crack growth under cyclic stresses and final

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failure due to crack coalescence [2]. In Ti-alloys 70–80% of total life is spent to initiate a crack and hence accurate estimate of number of cycles to crack initiation dictates the overall accuracy of predicted life. Crystal plasticity based finite element simulations in conjunction with a physically motivated crack initiation law can be used to accurately predict crack initiation in these alloys. However single time scale simulations for large number of cycles till crack initiation, employing conventional time integration schemes [12], can prove to be computationally prohibitive. In the single time integration schemes, each cycle is resolved into an appropriate number of time steps, over which integration is performed. In crystal plasticity calculations, a high resolution in the time steps is required for each cycle throughout the loading process, often leading to exorbitant computational requirements. Accelerated time integration schemes have been devised to perform the integration in an efficient manner for computational benefit.

Some of the existing accelerated time integration schemes are extrapolation based techniques, asymptotic expansion based methods and almost periodic temporal homogenization (APTH) operator based method. In extrapolation based methods [13–15], 3-D crystal plasticity simulations are performed for a small number of cycles and then the response variables are extrapolated to make fatigue life predictions. Extrapolation of local micro-structural variables can have considerable error and this can result in inaccurate prediction of number of cycles to crack initiation. The crystal plasticity variables display dual time scale characteristics under cyclic loading conditions, consisting of a high frequency oscillatory response (fine scale) and a low frequency monotonic response (coarse scale). This provides the basis to use temporal multiscale methods to decouple the coarse and fine scale response. The coarse scale response can then be integrated with larger time steps (in order of cycles) to attain significant computational benefit. Asymptotic expansion based methods and APTH operator based method falls under the category of multi-time scale methods. Asymptotic expansion based methods [16–18] assume scale separation and the crystal plasticity variables are expanded in an asymptotic series. The rate equations are modified based on different orders of contribution and integration of cycle-averaged variables are performed for computational benefit. These methods assume local periodicity or near periodicity and fails for reversible loading situations ($R\rightarrow -1$) where plastic oscillators are dominant. In APTH operator based method [19], almost periodicity of response variables are assumed and an operator is defined which satisfies the temporal periodicity condition in a weak sense for almost periodic variables. A staggered global–local approach is used to integrate the coarse scale variables for computational advantage. The strong non-linearity existing in crystal plasticity model for Ti-alloys makes the APTH operator based method to be unstable and hence cannot be used. The wavelet based multi-time scale method for cyclic simulations of polycrystalline alloys developed in [20] overcomes the drawbacks present in the existing accelerated time integration schemes. There is no assumption on the local periodicity of the variables and an implicit integration scheme is developed which is stable for strongly non-linear crystal plasticity model of Ti-alloys. This method is extended in the current work to perform finite element simulations of Ti-micro-structure under dwell fatigue loading with large time periods.

The organization of the paper is as follows. Section 2 describes the crystal plasticity model for Ti-alloys (Ti-6Al, Ti-6242). The existing accelerated time integration methods and their shortcomings are discussed in Section 3. The wavelet transformation based multi-time scale method is described in Section 4. Numerical results are presented in Section 5 to demonstrate the accuracy of the wavelet based method and also the ability to perform crystal plasticity based finite element simulations for large number of cycles. The paper is concluded in Section 6.

2. Crystal plasticity model for Ti-alloys

In crystal plasticity theory, the plastic deformation in polycrystalline alloys happens through slip on different slip systems [5]. The number of slip systems and their strength depends on the morphological and crystallographical characteristics of the micro-structure. Hence the micro-structural effect on the deformation of polycrystalline material is captured through crystal plasticity based models. The micro-structure of Ti-alloys (Ti-6Al, Ti-6242) is composed of primary α grains and transformed $\alpha+\beta$ colonies. The primary α grains have a hexagonal close packed (*hcp*) crystal lattice structure and is strongly anisotropic [6]. The transformed $\alpha+\beta$ colonies consist of alternate lathe of *hcp* lattice (α phase) and symmetric body centered cubic (*bcc*) lattice (β phase) [7]. The *hcp* crystal structure consists of three $\langle a\rangle$ basal slip systems $\{0\,0\,0\,1\}\langle 1\,1\,\bar{2}\,0\rangle$, three $\langle a\rangle$ prismatic slip systems $\{1\,0\,\bar{1}\,0\}\langle 1\,1\,\bar{2}\,0\rangle$, six $\langle a\rangle$ pyramidal slip systems $\{1\,0\,\bar{1}\,1\}\langle 1\,1\,\bar{2}\,0\rangle$, 12 $\langle c+a\rangle$ first order pyramidal slip systems $\{1\,0\,\bar{1}\,1\}\langle 1\,1\,\bar{2}\,3\rangle$ and six $\langle c+a\rangle$ second order pyramidal slip systems $\{1\,1\,\bar{2}\,2\}\langle 1\,1\,\bar{2}\,3\rangle$. The strongly anisotropic and orientation dependent plastic behavior of the α phase is due to the vastly different slip system resistances. The basal and prismatic $\langle a\rangle$ slip systems have the lowest resistance and are most favorable for slip activity, whereas the pyramidal $\langle c+a\rangle$ slip systems have the highest resistance showing no slip activity at room temperature. A transversely isotropic elastic tensor, with five independent constants, is used to model the elastic behavior of the α phase in these alloys. The β phase in these alloys have a cubic symmetry requiring three independent constants to model the elastic response and 48 slip systems divided into three families, $\{1\,1\,0\}\langle 1\,1\,1\rangle$, $\{1\,1\,0\}\langle 1\,1\,2\rangle$ and $\{1\,1\,0\}\langle 1\,2\,3\rangle$, to model the plastic response.

In crystal plasticity model, the total deformation gradient at a material point is multiplicatively split into an elastic and plastic part [6,7] as shown in Eq. (1). The elastic part of the deformation gradient $\mathbf{F^e}$ captures the stretching and rotation of the lattice. Plastic deformation happens through crystallographic slip on different slip systems and is captured through the evolution of the plastic deformation gradient $\mathbf{F^p}$ as shown in Eq. (2):

$$\mathbf{F}=\mathbf{F^e}\mathbf{F^p} \tag{1}$$

$$\dot{\mathbf{F}}^{\mathbf{p}}\mathbf{F}^{\mathbf{p}-\mathbf{1}}=\sum_{\alpha}\dot{\gamma}^{\alpha}\mathbf{S}_{\mathbf{0}}^{\alpha} \tag{2}$$

Here $\dot{\gamma}^{\alpha}$ is the slip rate on different slip systems and $\mathbf{S}_{\mathbf{0}}^{\alpha}$ is the Schmid tensor. The Schmid tensor is formed from the slip direction $\mathbf{m}_{\mathbf{0}}^{\alpha}$ and slip plane normal $\mathbf{n}_{\mathbf{0}}^{\alpha}$ in the reference configuration such that $\mathbf{S}_{\mathbf{0}}^{\alpha}=\mathbf{m}_{\mathbf{0}}^{\alpha}\otimes\mathbf{n}_{\mathbf{0}}^{\alpha}$. A power law is used to model slip rate on different slip systems as

$$\dot{\gamma}^{\alpha}=\dot{a}\left|\frac{\tau^{\alpha}-\chi^{\alpha}}{g^{\alpha}}\right|^{1/m} \tag{3}$$

Here $\dot{a}$ is a reference slip rate, τ^{α} is the resolved shear stress on the slip system, χ^{α} is the back stress, g^{α} is the slip system resistance and m is the power law exponent. The resolved shear stress on a slip system is related to the 2nd Piola–Kirchoff (PK2) stress as shown in Eq. (4). A hyper-elastic law is used to obtain the PK2 stress from the work conjugate Lagrange–Green strain tensor and is shown in Eq. (5). The evolution of slip system hardness is shown in Eq. (6) where h^{β} is the strain hardening rate due to self-hardening and $q^{\alpha\beta}$ is a matrix describing latent hardening. The evolution of back stress on a slip system depends on the slip rate on that slip system [21] and is shown in Eq. (7), where c and d are the direct hardening and dynamic recovery coefficient respectively:

$$\tau^{\alpha}=\mathbf{F^{eT}}\mathbf{F^{e}}\mathbf{T^{*}}:\frac{1}{2}(\mathbf{S}_{\mathbf{0}}^{\alpha}+\mathbf{S}_{\mathbf{0}}^{\alpha\mathbf{T}}) \tag{4}$$

$$\mathbf{T^{*}}=C:\mathbf{E^{e}}\quad\text{where }\mathbf{E^{e}}=\frac{1}{2}\left(\mathbf{F^{eT}}\mathbf{F^{e}}-\mathbf{I}\right) \tag{5}$$