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Prediction of crack initiation sites in alpha Ti-alloys microstructures under dwell-fatigue using Cellular Automaton simulation method

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ABSTRACT

The elastoviscoplastic behavior of α Ti-alloys microstructures is simulated under dwell-fatigue loading in order to identify the favorable crack initiation sites. To aim this goal, a mathematical model is developed using Cellular Automata (CA) approach. Each α Ti-alloy microstructure is presented with a Cellular Automaton formed of 900 and 10,000 cells where each cell represents a hexagonal close packed (HCP) grain of a polycrystalline microstructure. In order to describe a non-textured microstructure, each cell was associated with a randomly distributed crystallographic orientation. The medium in the CA model was built using the six first-degree neighbor cells. Each cycle of dwell-fatigue loading is simulated by three steps: load, creep and unload using the averaged stress–strain fields in all cells. An adapted elasto-plastic Eshelby localization approach is used to reach the local strains and stresses in each cell. The elastoplastic behavior of cells during the load step is simulated using a linear isotropic hardening model while a time dependent elastoviscoplastic model is used for the simulation of the cells' behavior during the creep step. The unload step is assumed to be elastic and residual stresses were calculated at the end of each load cycle and stored for the next cycle. Simulations were run for 3000 dwell-fatigue cycles on three different non-textured microstructures. Stress–strain fields at macro/microscopic scales dwell time effect and critical cells which can be favorable for crack initiation were investigated. The results obtained by the CA model are in accordance with experimental observations found in the literature in terms of stress–strain distributions, crack initiation sites, dwell time effect and the effect of microstructures dispersion. Distribution of residual stresses and neighbors' effects are finally investigated and discussed.

1. Introduction

Since the 1950's, the aerospace industry became interested in using titanium alloys for the manufacturing of turbo-machines' components because of their interesting mechanical properties, low density, corrosion resistance and their high temperature performance. The experimental studies [1–4] have shown that the lifetimes of theses alloys under dwell-fatigue can be significantly reduced (up to 5 times) compared to those under normal fatigue due to the introduction of a hold period at peak stress. This phenomenon is generally called dwell sensitivity. These studies have shown the different factors such as peak applied stress, dwell time, and microstructure can influence the dwell sensitivity. There are general agreements in the literature that dwell sensitivity happens at ambient temperature and it increases by increasing the maximum applied stress and also the dwell time. However, the microstructure was found to have dominant effect on dwell sensitivity due to the presence of multi-forms (crystallographic phases and orientations, size and morphology of grains) and multi-scales (micro/meso/macroscopic) heterogeneities in Ti-alloys. In fact, the dwell-fatigue behavior of a mechanical part made of titanium alloys can be widely dispersed from one place to another due to these different heterogeneities [5].

Numerous studies have proven that dwell-fatigue promote internal crack initiations which lead to quasi-cleavage facets observed on the rupture sites [1,4,6]. Theses facets can be categorized in initiation and propagation facets. Initiation facets, which are the main concern of this paper, are generally occurring on the basal planes of α primary grains [6]. Damage mechanisms explaining facet formation can be divided in two categories. First, a mechanism for that the formation has been proposed on the basis of a crack initiation in primary α grains with their basal plane perpendicular to the loading axis [1,2,4,7,8]. For this mechanism, the maximum normal stress applied to the basal plane is the main mechanical criteria for crack initiation. Second, other studies have

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shown that crack initiation sites are not perfectly normal to the loading axis [9–12]. The analyses conducted by Sinha et al. on three rupture sites of dwell-fatigue show that the facets were formed on the basal planes oriented 14–20° relative to the loading direction. In addition, the experimental results of Bridier et al. [13–16] cannot be explained only by the previous mechanism. In fact, their observations show that initiation sites are inclined relative to the loading axis, indicating not only a high normal stress favorable to cleavage, but also a high shear stress on the basal system, therefore, a favorable slip system. Thus, the crack initiation is considered to be the result of a dual condition of plasticity and normal stress. This mechanism can explain both ductile and brittle evidences observed on facets sites. This paper focuses on the second mechanism to explain the facet formation.

Traditional methods used to calculate the fatigue life are not suitable for predicting the lifetime of titanium parts under dwell-fatigue due to the complex factors influencing the dwell effect. Therefore, these parts have to be replaced before the end of their real life as a precautionary and safety measures. This is a costly process that enhances the need for the development of numerical tools that allow, at first, to understand the physical phenomena hidden behind this significant reduction of lifetime and eventually to predict the lifetime of these alloys under cold dwell-fatigue loading.

In order to do so, discrete mathematical models based on CA method will be used in this study. The CA model was introduced in late 1950s by Ulam and Neumann to calculate the motion of a liquid by considering it as a group of cells [17]. In their model, the motion of each cell as related to the behavior of its neighboring environment. Later, John Conway developed a computer game called "game of life" based on the CA method. In this game the color of each cell changes to white or black based on its neighboring cells' colors. In general, the CA method is simple to use while it can manage high level of complexity and diversity of behaviors between its constituent cells and can be widely used in mathematics, physics and material science.

In this paper a CA model based on simple hypotheses is developed with two principal objectives: (1) modeling the local and the global elastoviscoplastic behavior of α Ti-alloy microstructures under dwell-fatigue loading using the CA method. This part aims to give better insights about the influence of microstructural heterogeneities on the stress–strain localization and local plastic strain accumulation; (2) studying the ability of the CA model in identifying the favorable crack initiation sites in different crystallographic configurations according to different damage criteria.

The CA method was used in numerous microstructure studies in material science, for example, Montheillet et al. [18] used the CA model to study the micromechanical behavior of two linearly viscous phases of a heterogeneous material. The CA method was also used for modeling the static/dynamic recrystallization process [19–22], simulating the phase transformation during the heating process [23] and also to model the solidification process [24] and the motion of grain boundaries in polycrystalline materials [25]. Boutana et al. [26,27] used CA models to simulate the cold creep behavior of Ti-alloys under creep and dwell-fatigue loading. Recently, Pourian et al. developed two CA models to simulate micromechanical behaviors of α Ti-alloys microstructure in elasticity and plasticity, respectively [28,29].

Similar works have been done in FE by different authors to predict High Cycle Fatigue (HCF) response in Ti-alloy microstructures. Przybyla et al. [30,31] developed a microstructure-sensitive extreme value probabilistic framework and applied it to duplex Ti–6Al–4V to identify the driving forces for fatigue surface and subsurface crack formation. The work demonstrates that primary alpha grains with a basal Schmid factor between 0.45 and 0.5 have a higher probability of accumulating large cyclic plastic strain. The model do not explain why the dwell-fatigue fracture facets observed are systematically found to be oriented between 10° and 15° [32]. Dunne and Rugg [32] also developed a crystal plasticity based model to investigate the conditions necessary to nucleate a quasi-cleavage facet in near-alpha HCP titanium alloys under cold-dwell fatigue. Based on their study, a "rogue grain combination" (a hard grain with its basal plane perpendicular to the loading direction surrounded by two soft grains) would be the preferential site to form a crack with a facet feature. Nucleation sites with facets perpendicular to the loading axes are again expected according to this model. More recently, Anahid et al. [8] developed a FE crystal plasticity-based crack nucleation model to simulate dual-phase titanium alloys undergoing dwell-fatigue loading at room temperature. Their model predicts the number of necessary cycles to initiate a crack, as well as the characteristics of the local site by using a criterion based on evolving variables and dislocations piled up at grain boundaries. Based on their study grain boundaries play an important role as the nucleation would take place due to and excessive dislocations piled up in a soft grain that would initiate a wedge type of micro-crack in an adjacent hard grain. According to their model, the non-local plastic strain gradients in the neighboring soft grains control the crack nucleation. The higher is the gradient, the lower is the local effective stress required for crack initiation.

The present paper takes a different type of approach and tries to predict the potential quasi-cleavage facet formation sites using a CA model. A particular attention is put on trying to understand why experimental nucleation site results display incline facets (10–20°) rather than perfectly perpendicular ones as suggested by the above models.

The CA model is an interesting and complementary alternative method for microstructure modeling compared to other simulation methods like Self-Consistent (SC), Monte-Carlo (MC) and Finite Element (FE). It allows studying the effect of the heterogeneous surrounding mediums present in polycrystalline materials that cannot be studied using the SC method due to the fact that the surrounding medium in the SC approach is assumed to be homogeneous for all grains resulting in average behavior rather than documenting extreme behavior cases, i.e., the one of particular criteria in fatigue. Large number of cells with complex behaviors under large number of cycles can be simulated using the CA method in a short period of time. This kind of simulation would be very costly in term of calculation time and informatics materials needed in FE method.

The CA model developed in this study simulates three non-textured α Ti-alloy microstructures of 900 cells. Each cell is associated with a specific crystallographic orientation and mechanical properties. In this study, the dwell-fatigue loading is decomposed in three steps: load, peak stress hold period and unload. Dwell-fatigue simulations were carried out for 3000 cycles. Stress–strain behaviors at both macroscopic and microscopic scales were studied for three different hold period. Critical cells which can be favorable for crack initiation are identified and discussed. The results of the CA model are compared with overall experimental results found in the literature. For the three studied microstructures, the CA model gave acceptable results compared to experimental observations in term of stress–strain localization, grains with crack initiation potential and the dwell time effect. Residual stresses and neighbors' effects are also investigated and discussed.

2. Presentation of the CA model

In their previous works, the authors developed two models based on CA method to simulate the micromechanical behavior of α Ti-alloys microstructures under monotonic loadings in