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Discrete dislocation and crystal plasticity analyses of load shedding in polycrystalline titanium alloys

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ABSTRACT

The focus of this paper is the mechanistic basis of the load shedding phenomenon that occurs under the dwell fatigue loading scenario. A systematic study was carried out using a discrete dislocation plasticity (DDP) model to investigate the effect of crystallographic orientations, localised dislocation behaviour and grain combinations on the phenomenon. Rate sensitivity in the model arises from a thermal activation process at low strain rates, which is accounted for by associating a stress- and temperature-dependent release time with obstacles; the activation energy was determined by calibrating an equivalent crystal plasticity model to experimental data. First, the application of Stroh's dislocation pile-up model of crack nucleation to facet fracture was quantitatively assessed using the DDP model. Then a polycrystalline model with grains generated using a controlled Poisson Voronoi tessellation was used to investigate the soft-hard-soft rogue grain combination commonly associated with load shedding. Dislocation density and peak stress at the soft/hard grain boundary increased significantly during the stress dwell period, effects that were enhanced by dislocations escaping from pile-ups at obstacles. The residual stress after dwell fatigue loading was also found to be much higher compared to standard fatigue loading. Taylor (uniform strain) and Sachs (uniform stress) type assumptions in a soft-hard grain combination have been assessed with a simple bicrystal DDP model. Basal slip nucleation in the hard grain was found to be initiated by high stresses generated by strong pile ups in the soft grain, and both basal and pyramidal slip nucleation was observed in the hard grain when the grain boundary orientation aligned with that of an active slip system in the soft grain. The findings of this study give new insight into the mechanisms of load shedding and faceting associated with cold dwell fatigue in Ti alloys used in aircraft engines.

1. Introduction

Dwell sensitivity of hexagonal close packed (HCP) α-Ti alloys has been a concern of the aero industry for decades (Adenstedt, 1949; Whittaker, 2011). Representative loading histories of low-cycle fatigue and low-cycle dwell fatigue are shown schematically in Fig. 1. Dwell fatigue is believed to cause the early failure of highly stressed components of gas turbines, such as discs and fan blades (Whittaker, 2011). It has been established that facet fracture, which is the development of a

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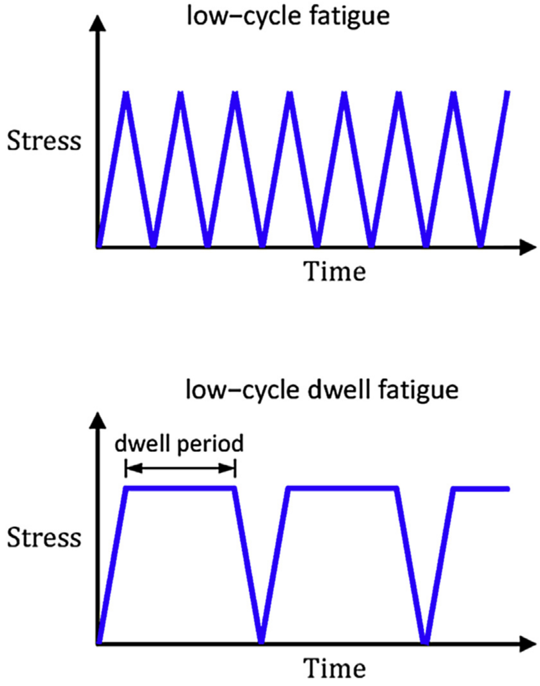

Fig. 1. Schematic illustration of low-cycle fatigue and low-cycle dwell fatigue loading histories.

micro-crack at the grain scale, is often found to be associated with loading that involves a stress-hold (dwell) at room temperature (Sinha et al., 2006). The faceting, particularly when it occurs in a large grain, may lead to a short lifetime, which manifests as dwell sensitivity of the alloy. Early observations, both experimental (Bache et al., 2010; Hasija et al., 2003; Sinha et al., 2006) and analytical (Bache et al., 1997; Bridier et al., 2009; Dunne et al., 2007a, 2007b; Evans and Bache, 1994; Ghosh and Anahid, 2013; Przybyla and McDowell, 2011; Zhang et al., 2015), have shown that the facet crack nucleation process is largely dependent on a particular crystallographic orientation combination: a weakly orientated (soft) grain adjacent to a strongly orientated (hard) grain with respect to the loading direction, referred to as a *rogue* grain combination. However, the mechanistic basis of this important phenomenon is not yet fully understood.

Hasija et al. (2003) reported creep of near-α Ti-6Al alloys under loading. The stress redistribution from the soft grain to the adjacent hard grain, which is known as load shedding, under stress dwell loading was also observed. The simulation results of Dunne and Rugg (2008) and Dunne et al. (2007a) also suggested that the presence of a stress dwell in each loading cycle causes higher damage compared to loading with a strain hold. In 1954, Stroh (1954) established a model to quantify the mode I opening stresses caused by a dislocation pile-up at a grain boundary along possible crack propagation planes in an adjacent grain. This model was further developed and utilised by Bache (1999, 2003) and Evans and Bache (1994) to understand the fatigue performance of titanium alloys. The effects of microstructure and morphology were also discussed systematically by Dunne et al. (2007a, 2007b) and Zhang et al. (2015). However, all of those analyses were conducted at the crystal level, hence cannot provide insight into the dislocation activity within grains or at grain boundaries. If the Stroh method of crack nucleation is indeed occurring in dwell fatigue, then it is important to carefully quantify and understand the dislocation activity near the soft-hard grain boundaries.

Discrete dislocation plasticity (DDP) is a modelling technique in which the motion of individual dislocations is explicitly captured (Van der Giessen and Needleman, 1995). However, classical two-dimensional DDP (Van der Giessen and Needleman, 1995) does not account for thermally activated processes, particularly the escape of dislocations pinned at obstacles via climb or local jog formation, hence classical DDP does not predict rate sensitivity at the low strain rates ($10^{-5}\mathrm{s}^{-1} \le \dot{\varepsilon} \le 10^{0}\mathrm{s}^{-1}$) that are associated with the Ti dwell fatigue problem. In this study, we use a mechanistic formalism that incorporates thermally activated dislocation escape (Zheng et al., 2016) into the classical DDP model. A time parameter is assigned to each obstacle that characterises how long it takes a dislocation pinned at that obstacle to overcome the associated energy barrier, hence making a successful escape attempt. The probability of successful attempts is governed by the Gibbs free energy of activation which can be expressed as the summation of the Helmholtz energy and the work done by the external stress field (Gibbs, 1969). The reverse jump from the new equilibrium position is also considered (Dunne et al., 2007a).

In this paper, we aim to provide a systematic analysis of the plastic response of polycrystalline HCP crystals under different loading conditions. A polycrystalline crystal plasticity (CP) model is used to obtain values of the critical resolved shear stress (CRSS) and activation energy associated with dislocation escape from obstacles by calibrating against experimental rate sensitivity results of a Ti-6Al alloy (Hasija et al., 2003). The parameters obtained from the CP calibrations are then used in