Microstructural effects on strain rate and dwell sensitivity in dual-phase titanium alloys

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In this study, stress relaxation tests are performed to determine and compare the strain rate sensitivity of different α–β titanium alloy microstructures using discrete dislocation plasticity (DDP) and crystal plasticity finite element (CPFE) simulations. The anisotropic α and β phase properties of alloy Ti-6242 are explicitly included in both the thermally-activated DDP and CPFE models together with direct dislocation penetration across material-interfaces in the DDP model. Equiaxed pure α, colony, Widmanstatten and basketweave microstructures are simulated together with an analysis of the effect of α grain size and dislocation penetration on rate sensitivity. It is demonstrated that alloy morphology and texture significantly influence microstructural material rate sensitivity in agreement with experimental evidence in the literature, whereas dislocation penetration is found not to be as significant as previously considered for small deformations. The mechanistic cause of these effects is argued to be changes in dislocation mean free path and the total propensity for plastic slip in the specimen. Comparing DDP results with corresponding CPFE simulations, it is shown that discrete aspects of slip and hardening mechanisms have to be accounted for to capture experimentally observed rate sensitivity. Finally, the dwell sensitivity in a polycrystalline dual-phase titanium alloy specimen is shown to be strongly dependent on its microstructure.

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1. Introduction

Dual-phase α–β titanium alloys are widely used in the aeronautical, marine, biomedical implants and sporting goods industries due to their high specific strength, fracture toughness, weldability and corrosion resistance [1]. Nevertheless, these alloys have been shown to be susceptible to fatigue failure under load dwell conditions at ambient temperatures (T < 0.3T_m), a failure mechanism referred to as cold dwell fatigue failure. Analysis of the failure surface has shown the presence of quasi-cleavage facets occurring perpendicular to the applied principal stress direction with near basal α orientations [2–4]. Considering the anisotropy of the HCP α crystal, these observations have been partly explained using the Stroh model [5], suggesting that a dislocation pile-up at the grain boundary in a well-oriented prismatic, soft grain can lead to the build-up of a high stress state in an adjacent basal-oriented, hard grain which can cause facet nucleation [3,6,7]. In order to address the dwell sensitive nature of the failure mechanism, Bache et al. (1997) hypothesised that creep operating during dwell increases slip accumulation at the soft-hard grain boundary, leading to more stress redistribution into the hard grain [7], a phenomenon referred to as ‘load shedding’ [8].

In addition to the particular soft-hard rogue grain combination, morphological effects have also been suggested to contribute to dwell fatigue failure. Recently, a comprehensive experimental study looking at the dwell sensitivity of alloys Ti-6Al-2Sn-4Zr-xMo with x = 2 to 6 has been carried by Qui et al. (2014) [9]. The results of this study showed that a number of changes occur as the Mo content (which is a β-stabiliser) increases from 2% to 6%: the α grain orientation distribution becomes more homogenised, the prior-β grain size decreases, and, for a similar thermomechanical processing route, the microstructure can change from colony microstructure in Ti-6242 to Widmanstatten/basketweave microstructure in Ti-6246. Crucially, for these microstructures, the dwell sensitivity decreased from Ti-6242 to Ti-6246. In general, experimental studies have shown that rate sensitivity decreases in the order of equiaxed primary α, colony to...
Widmanstatten/basketweave microstructures [10–12] and with smaller α-lath thicknesses [13]. It has also been shown that the alloy yield strength follows a Hall-Petch type relationship with α-lath thickness [13,14]. These effects are considered to arise from the decrease in mean free path for slip [13], where the length-scale dependent impendence to slip arises from the α–β interface which has been investigated in detail by Mills and coworkers. Suri et al. (1999) [15] and Savage et al. (2001, 2004) [16,17] used micromechanical experimental techniques to show that there exists anisotropy in the creep and yield response of colony microstructures oriented for different prismatic and basal slip systems, attributing it to the ease of dislocation penetration across the α–β interface depending on the degree of alignment of slip directions in adjacent phases as determined by the Burgers Orientation Relationship (BOR) [18]. These studies suggest that the extent of slip transmission across the α–β interface, which is determined by the alloy morphology and texture, can play an important role in determining the yield and rate sensitive response of titanium alloys.

Thus, texture, morphology and atomic-level intrinsic dislocation mechanisms can be considered to affect the dwell sensitivity of dual-phase titanium alloys. Atomistic simulations or ab initio calculations can provide insights into the effect of alloy composition on intrinsic dislocation mechanisms [19] whereas continuum-based simulations have already confirmed the load shedding analysis for textures containing the rogue grain combination [8,20,21]. However, the effect of the particular α–β morphology has only recently been incorporated into simulations to investigate the effect of the exact alloy microstructure.

For this purpose, the material parameters of the constituent phases are required. Zhang et al. [22,23] have utilised combined micropillar stress relaxation testing and crystal plasticity finite element (CPFE) simulations to calibrate the intrinsic strength and strain rate sensitivity parameters for the individual α and β slip systems for alloy Ti-6242. Zhang and Dunne (2017) [24] incorporated these slip system-dependent material parameters into a CPFE model to specifically investigate microstructural effects on strain rate sensitivity. Using a colony microstructure, they found that β-lath orientation and β volume fraction (increased up to a maximum of 20%) have only a small effect on the material rate sensitivity. For basketweave microstructures, they reported that having a number of different α variants in the microstructure leads to a decrease in rate sensitivity. From this, the authors concluded that α–β morphology has a small effect on rate sensitivity whereas texture has a significant effect. Although increasing the extent of sample constraint by imposing periodic boundary conditions reduced the strain rate sensitivity (SRS) coefficients observed in the CPFE modelling, the values obtained (~0.08) were still significantly higher than previously reported experimental values (~0.02) for large-scale polycrystalline titanium alloys [8]. This was considered to be caused by a lack of discrete aspects of slip being included in the model.

In order to capture discrete dislocation mechanisms relevant to dwell fatigue loading, Zheng et al. (2016) [25] have developed a planar discrete dislocation plasticity (DDP) model capable of simulating the deformation response of HCP crystals for a wide range of strain rates. High strain rate regimes (~ > 10^3 s^{-1}) are dominated by dislocation nucleation and viscous drag whereas low strain rate regimes, which are more relevant to dwell fatigue failure, are dominated by thermally-activated processes. Using this newly developed DDP formulation, Zheng et al. (2017) [26] showed there is increased load shedding for a rogue grain combination with dislocation penetration across grain boundaries than without, highlighting the importance of including discrete dislocation mechanisms in efforts to understand dwell fatigue sensitivity, since this insight had not been provided by previous CPFE studies. However, this DDP model assumed a homogenised material microstructure, only accounting for the actual alloy α–β morphology by calibrating different model material parameters for the alloys Ti-6242 and Ti-6246 to experimental results [27]. Therefore, microstructural effects on dwell sensitivity were not naturally captured by the model but only as a consequence of phenomenological calibration.

Only recently have discrete dislocation plasticity model parameters been calibrated for the individual α and β phases. Due to the particular plane-strain plasticity requirement for 2D-DDP, Zheng et al. (2018) [28] have utilised the CPFE model of Zhang et al. (2016) [23] which itself had been calibrated to experiments, to generate test specimens suitably oriented to fulfil the plane-strain condition. By comparing the DDP and CPFE simulations, Zheng et al. were able to obtain DDP model parameters for the individual α and β slip systems for alloy Ti-6242. In addition, the authors determined the stress required to transmit a dislocation across the α–β interface while showing that dislocation penetration had to be incorporated in the DDP model to suitably capture the dual-phase specimen behaviour.

With the work of Zheng et al. the state of the DDP field is now at a position to investigate microstructural effects on dwell sensitivity while including discrete plasticity and dislocation penetration mechanisms. This study aims to make initial headway into this objective. The thermally-activated DDP formulation of Zheng et al. (2018) [28] is used which explicitly includes dislocation penetration across the α–β interface and material heterogeneity of the α and β phases. The role of α–β morphology, crystallography of α variants, dislocation penetration and size effects in determining the material rate sensitivity are investigated in detail. The mechanisms elucidated by DDP are compared with those obtained from corresponding CPFE simulations to compare the insights provided by the two modelling techniques. Lastly, the effect of microstructure on the load shedding observed in a dual-phase polycrystalline specimen containing a rogue grain combination is investigated.

2. Methodology

Temperature and strain-rate dependent deformation of dual-phase titanium alloys has been simulated in both CPFE and DDP modelling by incorporating the mechanism of thermally-activated dislocation depinning from obstacles. CPFE model parameters for the individual α and β phase slip systems were obtained by Zhang et al. [22,23] by calibrating the simulations to micropillar compression experiments of single crystal α and dual-phase α–β micropillars taken from a Ti-6242 alloy. Zheng et al. (2018) [28] then utilised these CPFE results to calibrate DDP model parameters for Ti-6242 including the constituent phase material properties but also the stress required to cause dislocation penetration across the α–β interface. The CPFE and DDP model formulations and parameters of these studies are utilised in this work to simulate different alloy microstructures and compare the two simulation techniques. Both the CPFE and DDP models explicitly incorporate α and β phase properties, with the DDP model also including direct dislocation penetration across phase boundaries. The model formulations are detailed as follows.

2.1. Crystal plasticity finite element method

The total deformation gradient tensor \( F \) can be expressed as the product of its elastic \( F^e \) and plastic \( F^p \) components:
\[ F = F^e F^p \]  

From the kinematics of deformation, the rate of plastic deformation \( F^p \) is:

\[ F^p = \dot{I}^p F^p \]  

where \( I^p \) is the plastic velocity gradient given as:

\[ I^p = \sum_i \dot{\gamma}_i^p \mathbf{s}_i \otimes \mathbf{n}_i \]  

where \( \mathbf{s}_i \) and \( \mathbf{n}_i \) are the slip direction and slip plane normal respectively, and \( \dot{\gamma}_i^p \) is the plastic shear strain rate (or slip rate) for slip system \( i \). The general expression for the plastic shear strain rate is given by the slip rule (Orowan’s equation) in terms of the mobile dislocation density \( \rho_m \), the mean glide velocity \( v_g \) and the Burgers vector \( \mathbf{b} \) as:

\[ \dot{\gamma}_i^p = \rho_m v_g b \]  

The glide velocity incorporating thermally-activated mechanisms is taken from Dunne et al. (2007) [20]. For a given slip system, the glide velocity is:

\[ v_g = b v D \exp \left( -\frac{\Delta F}{kT} \right) \sinh \left( \frac{(\tau - \tau_c) \Delta \nu_{CP}}{kT} \right) \]  

where \( v_D \) is the Debye frequency of atomic vibrations, \( k \) the Boltzmann constant, \( T \) the absolute temperature, \( \Delta F \) the activation energy of the thermally-activated mechanism, \( \Delta \nu_{CP} \) the activation volume over which work is done by the effective stress field, \( \tau \) the resolved shear stress at a given position and \( \tau_c \) is the critical resolved shear stress of the slip system. Length-scale effects arise from the evolution of geometrically necessary dislocations (GNDs) but statistically stored dislocations (SSDs) are considered to have a constant density. The total mobile dislocation density \( \rho_m \) used in Eq. (4) is then given by the sum of the GND and SSD densities. From Busso et al. (2000) [29], the general form of the incremental change in the GND density \( \Delta \rho_{GND} \) for a given slip system is calculated as:

\[ \Delta \rho_{GND} = \frac{\Delta \nu}{b} \text{curl} [\mathbf{n} F^p] \]  

which is the density of GNDs required to represent the discontinuity in Burgers vector circuit arising between two time increments due to plastic strain gradients. The initial GND density is zero.

### 2.2. Planar discrete dislocation plasticity

Zheng et al. (2016) [25] developed a 2D discrete dislocation plasticity model incorporating thermally-activated mechanisms. They considered that dislocations can become pinned at point obstacles from which thermally-activated depinning can occur, with the frequency of successful forward jumps being \( \Gamma = \frac{v_D}{\tau_{obs}} \) where \( \tau_{obs} \) is the obstacle spacing along the dislocation line. The activation volume is defined here as \( \Delta V^{DDP} = \tau_{obs} b^2 \), giving the expression for the frequency of successful forward jumps as:

\[ \Gamma = \frac{v_D}{\tau_{obs}} \exp \left( -\frac{\Delta F}{kT} \right) \sinh \left( \frac{\tau_{dis} \Delta V^{DDP}}{kT} \right) \]  

The frequency of successful jumps can also be expressed \( \Gamma = \frac{v_D}{\tau_{obs}} \) such that the time constant \( \tau_{dis} \) for a dislocation pinned at an obstacle can be obtained after determining \( \Gamma \) from Eq. (7). If the dislocation pinned time exceeds \( \tau_{obs} \) and the shear stress on the dislocation \( \tau_{dis} \) exceeds the mean nucleation strength of the material, the dislocation is unpinned and allowed to glide freely again until it encounters another obstacle. The activation energy \( \Delta \nu \) is considered to be the same as that determined from CPF, but the source parameters and the activation volume \( \Delta V^{DDP} \) are fitting parameters that have recently been determined by Zheng et al. (2018) [28] for Ti-6242.

The free flight of dislocations is considered to be determined by a linear mobility law \( v_{dis} = f_i b \) where \( f_i \) is the Peach-Koehler force acting on a dislocation \( i \) and \( B \) is the drag coefficient. In order to account for material heterogeneity in the dual-phase titanium system, the superposition scheme proposed by O’Day and Curtin (2004) [30] is utilised. Each homogeneous material region is considered to be a separate discrete dislocation (DD) sub-problem with generic boundary conditions. The complete solution is given by the superposition of the individual DD-subproblems and a global finite element (FE) subproblem to account for the applied boundary conditions. Thus, the Peach-Koehler force on a dislocation \( i \) is given as:

\[ f_i^{(l)} = n_i^{(l)} \left[ \sigma_{\mathbf{n}} + \sum_j \sigma_{\mathbf{n}}^{(j)} + \sigma_{\mathbf{b}}^{(j)} \right] b_j^{(l)} \]  

where \( n_i^{(l)} \) is the normal to the slip plane containing the dislocation and \( b_j^{(l)} \) is the dislocation Burgers vector, with the (001) and (111) field solutions being used for the DD subproblem in which the dislocation lies. Point sources, acting as a 2D representation of Frank-Read sources, are randomly dispersed with a density \( \rho_p \) throughout the material on slip planes spaced 100b apart. Each source is prescribed a nucleation strength \( \tau_{nuc} \) from a Gaussian distribution with mean \( \tau_{nuc} \) and a standard deviation of 80 MPa. The nucleation time of a source is considered to be \( \tau_{nuc} \times 10 \) ns, i.e. proportional to the ratio of the source strength to the mean nucleation strength. Dislocation dipoles are nucleated if the resolved shear stress on the source is greater than \( \tau_{nuc} \) for the duration of the nucleation time. The point obstacles from which thermally-activated depinning occurs are randomly dispersed on the slip planes with a density \( \rho_{obs} \). The slip systems activated for plane-strain plastic deformation in BCC \( \beta \) phase and HCP \( \alpha \) phase together with the slip directions projected onto the plane of deformation are shown in Fig. 1. Each of the BCC beta phase, HCP alpha phase soft orientation and HCP alpha phase hard orientation are considered to be isotropic, linear elastic materials that constitute the separate DD sub-problems.

Slip transmission between adjacent phases is included by direct dislocation penetration across the \( \alpha - \beta \) material interface using the formulation of Li et al. (2009) [31] as illustrated in Fig. 2 (a). The leading dislocation in a pile-up at a material interface is able to penetrate across the interface into the adjacent phase if the work done by the stress state at the dislocation exceeds the combined energy barrier of the interface and the dislocation debris thus formed. Let the interfacial energy of the phase boundary be \( \gamma_{\alpha-\beta} \), the Burgers vector of the incoming dislocation in Phase 1 be \( \mathbf{b}_1 \) and of the dislocation debris \( \mathbf{b} \), then dislocation penetration occurs when:

\[ \tau_{dis} |\mathbf{b}_1|^2 \geq \tau_{pass} |\mathbf{b}_1|^2 = \gamma_{\alpha-\beta} |\mathbf{b}_1| + \mu (|\Delta \mathbf{b}|)^2 \]

where \( \tau \) taken to be the shear modulus of the phase from which transmission is occurring. The dislocation debris energy term incorporates within itself a geometric criterion that the energy of the debris increases with the magnitude of the Burgers vector.
difference. This implies that if there is a mismatch in the magnitudes of the Burgers vector in the adjacent materials or a misorientation in the incoming and outgoing slip-planes, a larger stress is required for dislocation penetration. Zheng et al. (2018) [28] determined the stress required to penetrate an $\alpha/\beta$ boundary as $\tau_{\text{pass}} = 5430$ MPa with no misorientation between the incoming and outgoing dislocation slip planes but a difference in Burgers vector magnitude of $|\Delta b| = 0.009$ nm. A conservative estimate of the phase boundary energy can be calculated from this $\tau_{\text{pass}}$ by considering dislocation penetration from the $\beta$ into the $\alpha$ phase giving $\gamma_{\alpha-\beta} = 1550$ mJ m$^{-2}$. There is an accumulation of dislocation debris as the number of transmission events increases. Dislocation re-emission from this debris is also allowed if it is geometrically and energetically feasible, further details of which can be found in Refs. [28,31]. In this work, the debris Burgers vector is considered to lie in the outgoing grain and is included in all calculations of displacement and stress.

For the finite element subproblems, non-uniform, linear triangulated meshes conforming to phase boundaries are generated using the open-source MATLAB code DistMesh by Persson and Strang (2004) [32] with an example mesh shown in Fig. 2(b). Convergent results were obtained with a largest element size of ~0.3 $\mu$m and a smallest element size such that at least three layers of elements existed across the $\beta$-lath thickness. Finally, a time-stepping scheme as outlined in Zheng (2016) [33] was utilised to simulate low strain rate deformation within practical time-scales. Briefly, a large and small time step of 0.5 ns and 100 ns respectively are defined. The large time step is used until any of dislocation nucleation, dislocation penetration or thermally activated dislocation depinning from obstacles occurs. Then the simulations are shifted to the small time step regime to achieve equilibrium in the dislocation structure, moving back to the large time step only if none of the aforementioned events occur during an increment and all dislocations have remained within a distance of 100 $b$ from their previous position. The CPFE and DDP model parameters determined by Zhang et al. [23] and Zheng et al. [28] respectively for Ti-6242 are utilised in this study and given in Table 1. The material elastic constants are given in Table 2.
3. Microstructural effects on rate sensitivity

Following the modelling techniques outlined above, a systematic parametric study is performed on the effect of different microstructural factors on material strain rate sensitivity (SRS). In this study, stress relaxation testing is used to quantitatively determine the specimen SRS coefficient. Stress relaxation testing is a well-established technique to characterise the rate sensitivity of a material with the added benefit for the purposes of this work that rate sensitivity can be obtained from one test, in contrast to other methods where multiple tests have to be performed such as the constant strain rate technique, leading to significant savings on computational time. For the specimen sizes and strain rates considered in this study, each simulation takes the order of a few weeks to complete. During stress relaxation, the specimen is held at a constant hold strain leading to zero total strain rate, with the strain rate sensitivity coefficient being obtained as $m = \frac{\log(\epsilon)}{\log(\epsilon_{\text{hold}})}$.

In this study, a 10 $\mu$m specimen is considered with a number of different possible microstructures. It should be noted that one such specimen represents one transformed prior-\(\beta\) grain and will be referred to as one microstructure. Within one such specimen, a number of \(\alpha\) and \(\beta\) laths can occur which are, to be precise, the individual grains. A simple geometric representation of the Widmanstatten microstructure, as shown in Fig. 3(a), is considered to be the control against which other microstructures are compared. For this study, the width of the individual \(\alpha\) ligaments $l_\alpha$ is fixed at 2.5 $\mu$m (unless otherwise stated) and the \(\beta\) volume fraction is fixed at 20% corresponding to reports from the literature for both properties [9,34].

The boundary conditions and loading regime for the stress relaxation testing are also shown in Fig. 3. The outer specimen boundaries are considered to be impenetrable for dislocations, unless otherwise stated. Specimens are loaded in tension at a strain rate of $10^{-2}$ s$^{-1}$ to a hold strain $\epsilon_{\text{hold}}$ of 1.5\% (unless otherwise stated) and then held at this maximum strain for 10 s. Stress relaxation occurs during the strain hold period which is recorded as the stress relaxation at the right specimen boundary where the loading is applied. A hold strain $\epsilon_{\text{hold}} = 1.5\%$ is chosen because a small hold strain is considered to be relevant for in-service loading.

For a plane-strain plasticity representation of the BCC \(\beta\)-phase, two soft and one hard \(\alpha\) variants exist which fulfill both the BOR and the plane-strain plasticity requirement. Assuming the \(\beta\) grain to be well oriented for slip, the grain orientations of the \(\alpha\) variants are shown in Fig. 4. Plasticity in the soft variants arises from prismatic slip whereas in the hard variant it arises from basal and pyramidal slip.

3.1. Effect of \(\alpha-\beta\) morphology and \(\alpha\) variants

In this section, the effect of \(\alpha-\beta\) morphology and the presence of different \(\alpha\) variants is analysed. The \(\alpha\) ligament width and \(\beta\) volume fraction are kept uniform for all morphologies. The different microstructures considered are shown in Fig. 5 together with the slip systems of the constituent \(\alpha\) and \(\beta\) grains. These microstructures are: pure \(\alpha\) well oriented for prismatic slip (Pure \(\alpha\);
colony with β-laths parallel to the primary slip direction (Colony k);
colony with β-laths perpendicular to the primary slip direction (Colony ⊥);
Widmanstatten microstructure with one α variant;
basketweave microstructure with a checker-board arrangement of
only soft α variants (BW s); and, basketweave microstructure with a
checker-board arrangement of soft and hard α variants (BW s+h).
The exact α grain orientations are also shown on Fig. 5 with the
same colour scheme as Fig. 4 to help identify α variants. The β
phase, if present, is always considered to be well oriented for slip
i.e. in the grain orientation shown in Fig. 4. Finally, parallel lines on
the figure indicate corresponding α1 || b1 slip directions.

The stress against time curves and the SRS coefficient m
obtained from the relaxation response are shown in Fig. 6(a) and (b)
respectively for the different microstructures. It can be observed
that the strain hardening and maximum stress reached before relaxation correspond inversely to the SRS coefficient obtained for the microstructures such that a discussion on one of these properties suffices. The SRS coefficient \( m \) decreases in the order of Pure \( \alpha \), Colony\(_{a} \), to similar values for Colony\(_{b} \), Widmanstatten and basketweave with soft variants (BW\(_{s} \)), and then finally to basketweave with both soft and hard variants (BW\(_{s,h} \)) having the lowest SRS coefficient. Pure \( \alpha \) microstructure has no material interfaces whereas the Colony\(_{a} \) microstructure has \( \beta \) laths impeding slip only for secondary slip systems, thus leading to a slightly smaller \( m \) from the Pure \( \alpha \) case. The Colony\(_{h} \) has an even lower SRS coefficient because there is impedance to slip in the primary slip direction by the \( \beta \) laths. Once there is strong impedance to primary slip (Colony\(_{h} \)), added impedance to secondary slip (i.e. the Widmanstatten microstructure) appears to have a negligible effect on the relaxation response such that both Colony\(_{a} \) and Widmanstatten microstructures have similar SRS coefficients. Thus, the differences in rate sensitivity of the Pure \( \alpha \), Colony\(_{a} \), Colony\(_{b} \), and Widmanstatten microstructure can be accounted for by an analysis of the mean free path for dislocations.

Comparison between Widmanstatten and the two basketweave cases, on the other hand, requires the consideration of other factors since these microstructures have a similar mean free path for dislocations. The SRS coefficient \( m \) is similar for the Widmanstatten and BW\(_{s} \) microstructures and much lower for the BW\(_{s,h} \) microstructure. Dislocation penetration across the \( \beta \) lath (i.e. going from \( a \rightarrow \beta \rightarrow a \)) should be reduced in both the basketweave microstructures due to the mismatch in the \( a_{1} \) directions of the \( a \) grains adjacent to a \( \beta \) lath as was shown in Fig. 5(e) and (f). However, the difference in the BW\(_{s} \) and BW\(_{s,h} \) microstructures is that BW\(_{s,h} \) has significantly less overall slip occurring in the specimen because of the inclusion of hard variants. Thus, Widmanstatten and BW\(_{s} \) have similar values of \( m \) because these microstructures have comparable propensity for plastic deformation whereas BW\(_{s,h} \) has a lower rate sensitivity because of significantly less total slip, without dislocation penetration being particularly important in this case.

The total slip distribution at the end of 10 s of stress relaxation for these different microstructures is shown in Fig. 7, with the total slip \( \zeta \) at a point being given by the summation of the resolved shear strain at that point on all slip systems [35]. A few long, unimpeded slip traces can be observed for the Pure \( \alpha \) and Colony\(_{a} \) cases, whereas a larger number of shorter traces being obstructed at the \( \beta \) laths are observed for the other microstructures indicating that slip has to be activated on more slip planes in these cases. Only a few instances of one-to-one correspondence of slip traces on either side of a \( \beta \) lath are observed, being an indication again that dislocation penetration may not be very significant. Finally, the difference in the extent of total slip is evident when comparing the slip traces of BW\(_{s} \) and BW\(_{s,h} \), where there is hardly any slip observed in the hard variants of BW\(_{s,h} \).

### 3.2. Role of dislocation penetration

To elaborate on the role of direct dislocation penetration, simulations are run on the Widmanstatten microstructure with either impenetrable or penetrable \( \alpha \rightarrow \beta \) material interfaces. Stress relaxation for each of these two types of interfaces are performed at two hold strains, \( \epsilon_{\text{hold}} = 1.5\% \) and 2.0\%. The stress against time response and SRS coefficients are shown in Fig. 8(a) and (b) respectively. It appears that dislocation penetration affects stress relaxation and rate sensitivity at the larger hold strain of 2\% but not at \( \epsilon_{\text{hold}} = 1.5\% \). It should also be noted that \( m \) increases with applied \( \epsilon_{\text{hold}} \) as expected. Since dislocation penetration is not considered to be a thermally-activated process in this model, it is not expected to directly contribute to time-dependent behaviour but rather indirectly through changes in the stress distribution. A larger dislocation density can build up in a specimen with penetrable material interfaces because dislocation penetration leads to reduced back stresses on dislocation sources. This effect is illustrated in the evolution of the dislocation density for the impenetrable and penetrable material interfaces shown in Fig. 9. With a higher dislocation density, there are more dislocations available to undergo thermally-activated processes. However, a significant difference in the dislocation density between the impenetrable and penetrable cases only appears to arise at the larger hold strain. Thus, the \( \alpha \rightarrow \beta \) material interfaces provide strong impedance to slip and are only overcome via dislocation penetration at larger hold strains when the stress in dislocation pile-ups is high enough.

### 3.3. Effect of a ligament width

The variation in average \( a \) grain size for different \( \alpha \rightarrow \beta \) titanium alloys has also been suggested to affect material rate sensitivity. Fig. 10 shows the stress relaxation response for Widmanstatten microstructures with \( l_{a} = 1.25, 2.5 \) and 5.0 \( \mu \)m and their corresponding SRS coefficients for stress relaxation tests performed at \( \epsilon_{\text{hold}} = 1.5\% \). Simulations are again performed for both impenetrable and penetrable material interfaces. It is observed that \( m \) increases with larger \( l_{a} \), in keeping with previous arguments for the mean free path for dislocations. It should also be noted that the relationship of the SRS coefficient against a ligament width appears to have a decreasing slope for the \( l_{a} \) values considered. However, more simulations should be performed to determine a statistically significant relationship. Lastly, for stress relaxation performed at
$\varepsilon_{\text{hold}} = 1.5\%$, including dislocation penetration does not appear to significantly affect rate sensitivity at the considered $\alpha$ ligament widths, with the only noteworthy yet small difference between impenetrable and penetrable material interfaces observed at $l_\alpha = 1.25 \mu m$.

3.4. Discussion on microstructural effects

These results indicate that different $\alpha - \beta$ morphologies, the inclusion of soft or hard $\alpha$ variants and changes in $\alpha$ grain size can lead to significant differences in the specimen rate sensitivity.
These differences can largely be explained by considering the mean free path for dislocations and the total propensity for plastic slip in the material, whereas dislocation penetration may not be as significant as previously considered for low hold strains. Qiu et al. (2014) [9] observed that with increasing Mo content in Ti-6246 \((x = 2 \text{ to } 6)\), the average \(\alpha\) grain size decreased and there was a more homogeneous distribution of \(\alpha\) variants. The results in this work demonstrate that both effects would lead to a reduction in rate sensitivity of the material and thus agree well with the experimental observation of Qiu et al. that dwell sensitivity decreased with these changes in microstructure from their Ti-6242 to Ti-6246. The smaller \(\alpha\) grain size leads to a reduced mean free path for dislocations, whereas a more homogeneous distribution of \(\alpha\) variants can lead to the presence of grains which are poorly oriented for slip (hard variants), thus reducing the total propensity for slip in the specimen. The homogeneous distribution is also important to prevent these poorly-oriented grains from occurring in clusters of common crystallographic orientations to prevent the formation of macrozones.

Zhang and Dunne (2018) [36] have recently argued that including multiple \(\alpha\) variants in a basketweave microstructure can lead to a reduction in the rate sensitivity of the material. The authors showed that a polycrystal specimen with multiple \(\alpha\) variants had significantly reduced plastic strain accumulation as compared to a specimen with no variants. Considering the discussion above, these findings can arise from an increased likelihood of some variants being poorly oriented for slip as an increasing number of variants are included. The results here show that it is important to consider precisely which variants, hard or soft, are being included.

As for dislocation penetration, Mills and coworkers [15,17] have used TEM observations on a deformed colony grain to demonstrate that there was a one-to-one correspondence in dislocations on either side of a \(\alpha\beta\) lath for a colony orientation with no misorientation between incoming and outgoing slip planes. The authors argued that this represented dislocation penetration. Importantly, these observations were made for samples deformed to large engineering strains of \(\sim 5\%\). The results in this study corroborate these experimental findings but also indicate that dislocation penetration may not be significant at small strains which are more likely to occur in-service for different applications.

### 4. Comparison with CPFE modelling

Using crystal plasticity finite element (CPFE) modelling, Zhang and Dunne (2017) [24] found that \(\alpha\beta\) morphology did not significantly affect the material rate sensitivity whereas the presence of different \(\alpha\) variants did. The authors also obtained SRS coefficients around \(-0.08\). The DDP parameters utilised in this study have been obtained by calibration to CPFE simulations, yet the SRS coefficients obtained in this study are around \(-0.02\), which is comparable to experimentally observed values [8]. The disparity in rate sensitivity observed between DDP and CPFE results is analysed in more detail in this section. Using the crystal plasticity finite element model detailed in Section 2.1, stress relaxation tests are performed on specimens with dimensions of \(10 \times 10 \times 2.5 \mu m\) with the front and back surfaces fixed to mimic plane-strain conditions and loading applied to the right boundary. Tests are performed for all the \(\alpha\beta\) microstructures, hold strains and \(\alpha\) ligament widths investigated previously using DDP. Both the DDP and CPFE model set-up and boundary conditions are shown in Fig. 11(a) for the Widmanstätten microstructure as an example. The SRS coefficients obtained for corresponding microstructures from CPFE and DDP are compared in the bar chart in Fig. 11(b). The solid lines are shown as a visual aid. The DDP results are shown only for penetrable material interfaces since the calibration of DDP material parameters to CPFE simulations included dislocation penetration [28]. It can be seen that the SRS coefficients obtained from CPFE are consistently higher than those obtained from DDP, although both modelling techniques lead to a similar trend between different...
It is hypothesised that this may be due to two key differences between the two models. Firstly, CPFE simulations assume a homogenised material uniformly capable of plastic deformation. Whereas, in DDP simulations, the discrete nature of plasticity is explicitly incorporated and, together with the statistical distribution of dislocation sources, implies that slip can become localised to certain slip planes that then dominate plastic deformation phenomena such as stress relaxation. Secondly, Zhang et al. (2016) [23] obtained the CPFE model parameters by calibrating to relatively unconstrained micropillar compression experiments and, as such, did not include hardening parameters and their associated effects (apart from the inclusion of GNDs which leads to the small size effect observed in Fig. 11). In DDP simulations, hardening arises naturally due to dislocation interactions e.g. back stresses arising from pile-ups formed at obstacles and material interfaces. Such hardening mechanisms can lead to a lower dislocation density developing in the specimen and also a lower frequency of thermally-activated dislocation depinning, both leading to a less rate sensitive material. In short, naturally incorporating the discrete nature of slip and hardening mechanisms leads to the lower SRS coefficients observed in DDP simulations as compared to CPFE.

In order to correctly interpret CPFE modelling results already in the literature, it is worth investigating the relative contributions of the discrete nature of slip and hardening mechanisms on rate sensitivity. In this section, simulations are performed for differently sized Pure α specimens undergoing well-oriented prismatic slip, again using both DDP and CPFE. For the DDP model, two types of specimens are considered, with the top and bottom boundaries as shown in Fig. 11(a) either being passivated or acting as free surfaces. The passivated boundaries imply that dislocations are not allowed to escape from the specimen; there is no actual elastic passivation layer of finite thickness affecting the specimen response. With free surfaces, dislocations are able to escape from the specimen leading to a specimen size effect because of statistical effects in the weakest source strength. With passivated boundaries, dislocations form pile-ups at the specimen boundary leading to a grain-size hardening effect. Thus, comparison of these two boundary conditions with CPFE results can allow us to partially decouple the effect of hardening from the effect of the discrete nature of slip in DDP in the context of rate sensitivity. Three specimens are considered with dimensions of 1.0 × 1.0 μm, 2.5 × 2.5 μm and 10 × 10 μm. Five realisations each are performed for the smaller two specimen sizes to obtain a statistically relevant, average response. Stress relaxation tests are performed at ε hold = 1.5% as before and the SRS coefficients obtained shown in Fig. 12. In comparison to both boundary conditions of DDP simulations, CPFE simulations consistently lead to a higher material rate sensitivity for each
specimen size and also to a smaller overall size effect. DDP with free surfaces has a lower value of SRS coefficient $m$ compared to the CPFE simulations, arguably because of the inclusion of the discrete and statistical aspects of plasticity. Introducing grain-size hardening further reduces the material rate sensitivity as seen from the case of DDP with passivated boundaries. These factors should be suitably considered when utilising CPFE modelling to investigate material rate sensitivity.

5. Load shedding in a polycrystalline sample

Cold dwell fatigue failure of titanium alloys is a major concern in aero-engine applications, arising from quasi-cleavage facet nucleation under load dwell conditions. Facet nucleation has been linked to load shedding in a rogue grain combination which refers to the redistribution of load from soft grains to an adjacent hard grain. Load shedding during the dwell period is directly associated with the rate sensitivity of the material, being exacerbated by a more rate-sensitive material. In this section, the effect of microstructure on load shedding observed in a polycrystalline specimen containing a rogue grain combination is investigated. In particular, the effect of the $\alpha - \beta$ morphology of the soft grains is analysed considering that, for a similar thermomechanical processing route, Qiu et al. (2014) obtained a colony microstructure for alloy Ti-6242 and a Widmanstätten/basketweave microstructure for Ti-6246. A realistic prior-\(\beta\) polycrystalline specimen of dimensions $10 \times 10 \mu m$ is generated using the VGRAIN software [37,38] with minimum, mean and maximum grain sizes of 3, 5 and 7 $\mu m^2$ respectively and a grain regularity coefficient of 0.95. Within this specimen, two different microstructures are considered: a colony microstructure representing a Ti6242-like alloy illustrated in Fig. 13(a) and a Widmanstätten microstructure representing a Ti6246-like alloy shown in Fig. 13(b). The intrinsic $\alpha$ and $\beta$ material properties and prior-\(\beta\) grain microstructure are considered to be the same for both microstructures. Within one prior-\(\beta\) grain, the $\alpha$ orientation is assumed to be uniform for all $\alpha$ ligaments. A rogue grain combination is considered at the centre of each specimen as highlighted in the figure. The $\alpha$ orientation in the rogue grain combination is shown in Fig. 13(c) and consists of an equiaxed primary $\alpha$ hard grain adjacent to either two soft colony grains for the Ti6242-like microstructure or two soft Widmanstätten grains for the Ti6246-like microstructure. All other prior-\(\beta\) grains undergo prismatic $\alpha$ slip (i.e. only consist of the soft $\alpha$ variant) and are randomly assigned both a grain orientation and a $\beta$ lath orientation. Dislocation penetration across material interfaces is included but the outer specimen boundaries are considered to be passivated as before. The 0.2% yield stress $\sigma_{0.2Y}$ of the Ti6242-like alloy with colony microstructure is determined under strain-controlled load shedding observed at a strain rate of $\dot{\varepsilon} = 10^{-2} s^{-1}$. This yield stress is found to be $\sigma_{0.2Y} = 1095$ MPa and is used as a reference for the dwell hold simulations. It should be noted here that the average prior-\(\beta\) grain size considered in the polycrystalline specimens shown in Fig. 13 is approximately $\sim 2.3 \mu m$, with $\alpha$ and $\beta$ ligament widths being even smaller. These grain sizes are generally much smaller than those occurring in physical dual-phase titanium alloys which are used in-service. The model specimen and grain sizes are chosen due to considerations of computational costs. Thus, there is a considerable grain size effect occurring in the specimens here, which is why large hold stresses are being used. However, the results that follow are still indicative of the relative dwell sensitivity of the microstructures.

The dwell loading regime is shown in Fig. 13(d) and consists of stress-controlled loading with a load up to a maximum hold stress $\sigma_{\text{hold}}$ in 12 s and then dwell at this stress for 12 s. The Neumann (force) boundary conditions are prescribed at the right specimen boundary. Tests are performed at two hold stresses $\sigma_{\text{hold}} = 0.85\sigma_{0.2Y}$ and $\sigma_{\text{hold}} = 0.95\sigma_{0.2Y}$. During dwell, the stress $\sigma_{\text{AX}}$ is calculated at the nodes of a $20 \times 65$ rectangular grid, the outer boundary of which is shown on the microstructures in Fig. 13, and the mean value of $\sigma_{\text{AX}}$ calculated at one position along $A - A'$ by averaging the stress at the 20 equally spaced horizontal grid-points at that $y$-position.

The mean $\sigma_{\text{AX}}$ stress at different positions along $A - A'$ in the specimen is shown in Fig. 13(e) for two different prior-\(\beta\) microstructures (a) colony and (b) basketweave. The stress is significantly lower at the outer boundaries of the specimen, where the load is redistributed from the hard grain to the soft colony grains. This effect is more pronounced in the colony microstructure due to the larger grain size and lower material rate sensitivity. In contrast, the basketweave microstructure shows a more uniform stress distribution across the specimen, with a higher stress at the centre due to the lower grain boundary area ratio.

The retention of the load shedding in a rogue grain combination is highlighted in the figure. The $\alpha$ orientation in the rogue grain combination is shown in Fig. 13(c) and consists of an equiaxed primary $\alpha$ hard grain adjacent to either two soft colony grains for the Ti6242-like microstructure or two soft Widmanstätten grains for the Ti6246-like microstructure. All other prior-\(\beta\) grains undergo prismatic $\alpha$ slip (i.e. only consist of the soft $\alpha$ variant) and are randomly assigned both a grain orientation and a $\beta$ lath orientation. Dislocation penetration across material interfaces is included but the outer specimen boundaries are considered to be passivated as before. The 0.2% yield stress $\sigma_{0.2Y}$ of the Ti6242-like alloy with colony microstructure is determined under strain-controlled load shedding observed at a strain rate of $\dot{\varepsilon} = 10^{-2} s^{-1}$. This yield stress is found to be $\sigma_{0.2Y} = 1095$ MPa and is used as a reference for the dwell hold simulations. It should be noted here that the average prior-\(\beta\) grain size considered in the polycrystalline specimens shown in Fig. 13 is approximately $\sim 2.3 \mu m$, with $\alpha$ and $\beta$ ligament widths being even smaller. These grain sizes are generally much smaller than those occurring in physical dual-phase titanium alloys which are used in-service. The model specimen and grain sizes are chosen due to considerations of computational costs. Thus, there is a considerable grain size effect occurring in the specimens here, which is why large hold stresses are being used. However, the results that follow are still indicative of the relative dwell sensitivity of the microstructures.

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The mean $\sigma_{\text{AX}}$ stress at different positions along $A - A'$ at the
beginning and end of hold for each microstructure is shown in Fig. 14(a) and (b) for $\sigma_{\text{hold}} = 0.85\sigma_{0.2Y}$ and in Fig. 14(c) and (d) for $\sigma_{\text{hold}} = 0.95\sigma_{0.2Y}$. The dotted lines indicate positions of the soft-hard prior-\(\beta\) grain boundaries. The load shedding phenomenon is seen to increase with hold stress as expected, but is not as significant as previously observed in studies with a homogenised microstructure [27,39], due to increased impedance to slip in the more physically-based microstructure considered here. Importantly, there is significantly more load shedding observed in the Ti6242-like microstructure than the Ti6246-like microstructure. The smaller mean free path for dislocations in the Ti6246-like microstructure prevents significant accumulation of slip during dwell at the soft-hard grain boundaries, leading to negligible load shedding. These results indicate that, for the same assumed alloy intrinsic phase properties or chemistry, different microstructures can lead to different dwell sensitivities.

It should be noted that the extent of load shedding observed in this section is a reflection of the effect of microstructure on rate sensitivity demonstrated earlier. From the results of the previous section, it is clear that a structure containing equiaxed pure \(\alpha\)-prismatic soft grains would experience even more load shedding than the Colony\(h\) soft grains considered here. Also importantly, changing the colony orientation of the soft grains may well switch off the observed load shedding; the Colony\(h\) soft grains are used to demonstrate a bad-case scenario. From the same argument, the introduction of hard variants in a basketweave soft grain would result in an even more dwell insensitive microstructure such that load shedding only occurs at much higher hold stresses. However, these hard variants would have to be distributed homogeneously throughout the soft grains or the overall specimen so as to avoid the formation of a cluster or macrozone of hard common crystallographic orientation. Thus, the overall microstructural dwell sensitivity of a dual-phase titanium alloy can be tuned by suitable design of microstructure.

### 6. Conclusions

In this study, the effect of microstructure on the strain rate sensitivity of a two-phase titanium alloy is investigated using discrete dislocation plasticity. The anisotropic \(\alpha\) and \(\beta\) phase properties of alloy Ti-6242 are explicitly included in the thermally-activated DDP model together with direct dislocation penetration across material-interfaces. Stress relaxation tests are performed to determine and compare the strain rate sensitivity of different specimens. The material interfaces arising from the presence of \(\beta\)-laths are found to provide strong impedance to slip, with dislocation penetration across the material interfaces being insignificant at low hold strains and only contributing to rate sensitivity at large hold strains. The simulations indicate that varying the mean free path for dislocations, e.g. by changing the \(\alpha-\beta\) morphology from pure \(\alpha\)-prismatic or well-oriented colony to Widmanstatten microstructures or by reducing the \(\alpha\)-ligament width within a given morphology, significantly influences the specimen rate sensitivity. Conversely, for a uniform dislocation mean free path, introducing hard variants into the texture considerably reduces the rate sensitivity because of a decrease in the total propensity to slip in the specimen. Thus, it can be concluded that both \(\alpha-\beta\) morphology and texture significantly influence the microstructural rate sensitivity of a two-phase titanium alloy.

Corresponding CPFE simulations are performed to compare the observed strain rate sensitivity coefficient \(m\) with DDP simulations. CPFE simulations demonstrate values of \(m \sim 0.05\), consistently higher than the corresponding DDP simulations where \(m \sim 0.02\) which is closer to experimentally observed values for polycrystalline dual-phase titanium alloys. It is demonstrated that the difference between DDP and CPFE arises due to two factors: one being the inclusion of discrete and statistical aspects of plasticity in DDP and the second being that hardening mechanisms are naturally incorporated in DDP via dislocation interactions with...


