Slip transfer across phase boundaries in dual phase titanium alloys and the effect on strain rate sensitivity

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A B S T R A C T

Dislocation transmission through α/β phase boundaries in titanium alloys is studied using integrated crystal plasticity (CP) and discrete dislocation plasticity (DDP) modelling techniques, combined with experimental micro-pillar compression test results. Direct dislocation transmission together with the nucleation of new dislocations ahead of a pile-up at an α/β interface, termed indirect slip transfer, are both assessed and their role in controlling microstructure-dependent strain rate sensitivity considered. A critical shear stress criterion for direct slip transfer across an α/β interface in Ti-6242 has been established by capturing the local slip penetration through the phase boundary using CP and DDP comparisons with experimental two phase micro-pillar compression. The competition between direct and indirect slip transfer has been investigated using a single Frank-Read source DDP model. Direct slip transfer is found to occur only under specific conditions which have been quantified. The strain rate sensitivity of dual phase titanium alloys is demonstrated to depend on average pile-up size which is significantly influenced by α/β morphology.

1. Introduction

Titanium alloys are used in critical components in the aerospace industry due to their high strength to weight ratio, excellent corrosion resistance and superior mechanical properties. They have been reported to show strong positive strain rate sensitivity (SRS) at ambient temperature (e.g. 20 °C) (Hasija et al., 2003) resulting in the observed creep and stress relaxation. Depending on the thermo-mechanical processing route, differing microstructures can be produced including equiaxed α (HCP) grains, α-β (BCC) colony structures, bimodal structures comprising colonies and equiaxed α, through to more complex Widmanstatten and basket weave (which is Widmanstatten-like, but includes multiple α-variants) structures. The resulting microstructural heterogeneity is found to affect the rate-dependent behaviour of these alloys very significantly. In particular, alloy Ti-6Al-2Sn-4Zr-2Mo (Ti-6242, near-α) is known to show strong stress redistribution under dwell fatigue loading which leads to dramatic lifetime reduction (the dwell debit) while Ti-6Al-2Sn-4Zr-6Mo (Ti-6246, α-β) is known to be dwell insensitive (Zheng et al., 2016a, 2017a), and the origin of these behaviours is increasingly argued to relate to microstructure as a result of the differing processing routes, as opposed to the chemistry differences. Qiu et al. (2014) studied the dwell response of Ti-624x (x = 2 to 6) alloys demonstrating significantly different creep responses decreasing from alloy Ti-6242 to Ti-4246. It was shown that the β phase volume fraction in Ti-6242 alloy was lower and the average α grain size larger compared to the Ti-6246 alloy. The reduction of α grain size potentially enhances the effect of α/β phase boundaries on the resulting creep response.
The study of dislocation interactions with grain boundaries can be tracked back several decades. Multiple techniques have been utilised in order to understand slip transfer across grain boundaries, such as nanoindentation (Britton et al., 2009), high-resolution electron backscatter diffraction (HR-EBSD) (Guo et al., 2014), low cycle fatigue loading (Joseph et al., 2018), pillar compression (Suri et al., 1999), atomistic (Sangid et al., 2011; Spearot and Sangid, 2014) and dislocation dynamics (Liu et al., 2012; Zheng et al., 2017b) simulations. Specifically for titanium alloys, Ambard et al. (2001) compared the deformation mechanisms of globular α grains and α-β colonies of Ti-6Al-4V alloy at 20 K. The presence of α/β interfaces led to a high density of dislocation pile-ups against the colony boundaries. Suri et al. (1999) investigated the role of slip transmission in single α-β colonies of Ti-5Al-2.5Sn-0.5Fe alloy at room temperature and its effect on the creep rate using transmission electron microscopy (TEM) characterisations. More recent work by Savage et al. (2004) provided detailed TEM analysis of the dislocation structure near α/β interfaces after compression of single α-β colonies of Ti-6242 alloy with different crystal orientations. In both of the aforementioned TEM work, dislocations are argued to transmit through the interfaces if similar Burgers vectors are observed on both sides of the boundaries. However, dislocation transfer through a boundary can be due to indirect transmission, i.e. the nucleation of Frank-Read sources located in front of a dislocation pile-up (Lee et al., 1989, 1990; Shen et al., 1986, 1988), or direct transmission, i.e. the leading dislocation of a pile-up directly transferring to a new slip plane on the opposite side of the boundary (Kondo et al., 2016; Zheng et al., 2017b). Direct dislocation transfer consists of the two stages of re-nucleation and dislocation emission as shown in Fig. 1. Considering an incoming dislocation with Burgers vector $b_1$, driven by the external stress and moving into a boundary or phase interface, the discontinuity caused by the dislocation acts as a dislocation source located at the interface, and if the local stress is high enough, a new dislocation $b_2$ may be generated and the external stress can drive the new dislocation emitting from the interface and continue to glide along the new slip plane. Due to the intrinsic difference in the incoming and outgoing dislocation Burgers vectors, a residual dislocation $\Delta b$ is generated and left at the interface until it is able to cause dislocation re-emission (Li et al., 2009). The overall Burgers vector is conserved during the whole process as described in Fig. 1c.

It remains difficult to differentiate between direct and indirectly transmitted dislocations from the relaxed dislocation structure in a deformed crystal. Recent work by Eftink et al. (2017) combining in situ and ex situ TEM straining experiments and molecular dynamics simulations demonstrated strain transfer through an interface accompanied by residual dislocation generation. Kondo et al. (2016) provided convincing evidence (through video data) of the observation of direct individual dislocation transfer through a low-angle grain boundary (GB) using in-situ TEM nanoindentation techniques on strontium titanate SrTiO$_3$ samples. Their results suggested that low-angle tilt grain boundaries slightly impeded the lattice dislocation motion but that direct slip transmission is possible. It is noted that there were no dislocation sources observed either side of the GB, and the dislocations were generated due to the lattice distortion around the tip of the indenter, hence indirect slip transmission is eliminated in this scenario. However, dislocation interaction with grain boundaries remains unclear when there is a competition between direct and indirect slip transfer. A recent review by Bieler et al. (2014) indicates that tracking local slip behaviour near grain boundaries is necessary in order to understand damage nucleation and evolution.

Jun et al. (2016) carried out micro-pillar testing on two phase Ti-6242 alloy to understand the local deformation mechanisms. The results revealed that both β volume fraction and the β morphology have significant effects on average micro-pillar stress response. Zhang et al. (2016) subsequently utilised crystal plasticity (CP) modelling to determine the anisotropic rate-dependent properties of α and β phases in Ti-6242 alloy by calibration against micro-pillar testing. As shown in Fig. 2, the crystal plasticity model is able to capture localised slip band development across the α-β interface as well as the overall stress-strain response. Their results also demonstrated the impediment to slip from increasing β lath thickness. Furthermore, Zhang and Dunne (2017) introduced the idea of ‘structural strain rate sensitivity’ by linking the average macroscale rate-dependent plasticity to polycrystal α-β morphology including β lath structure and α phase variants. The plastic strain development through the β lath as observed in Fig. 2b using crystal plasticity modelling might best be described as strain nucleation corresponding to indirect slip transfer: slip is initiated in the β phase due to the high stress developed at the phase boundary. Even though no constitutive law associated with direct slip transmission is implemented in the CP model, much of the observed deformation behaviour is successfully captured. However, the question remains how direct
Dislocation transmission affects the rate dependent plasticity of titanium alloys, and under what circumstances direct slip transfer plays a negligible role such that CP modelling is accurate enough to predict the local material response.

Discrete dislocation plasticity (DDP) modelling incorporating thermally-activated dislocation escape from obstacles and direct slip transmission through $\alpha/\alpha$ grain boundaries has been used by Zheng et al. (2017b) to study the load shedding phenomenon (stress redistribution from soft to hard grains during peak stress hold periods) in Ti-6242 alloy under dwell fatigue loading. The energy barrier for dislocation transmission through boundaries between $\alpha/\alpha$ grains was argued to be related to the static grain boundary penetration energies; grain boundary energy can be determined by molecular dynamics (MD) simulations. The results suggest that load shedding is enhanced when dislocation transmission is permitted. A key controlling mechanism with respect to load shedding in titanium alloys is the process of thermally activated dislocation escape from obstacles while dislocation-grain boundary penetration exacerbates the load shedding by increasing the size of dislocation pile-ups, but plays a secondary role. Sangid et al. (2011) quantified the energy barrier of direct dislocation transmission in a face-centered cubic material using molecular dynamics simulations. However, such methods are not yet capable of addressing $\alpha/\beta$ boundaries in titanium alloys because of the absence of interatomic potentials and the complexity of the atomistic structures at phase boundaries.

Extensive atomistic modelling work by Wang and co-authors (Wang, 2015; Wang et al., 2012) also provides excellent insights into understanding dislocation-grain boundary interactions. The results from single dislocation interactions with an FCC/BCC interface suggests that the direct slip transmission process consists of old dislocation absorption by the GB, new dislocation nucleation and dislocation emission. Furthermore, the slip transmission barrier is found to increase with decreasing interface strength (Wang et al., 2012). The interaction between a group of dislocations, i.e. a single pile up, and a grain boundary can induce a series of local reactions, such as direct slip transmission, GB sliding, GB migration etc. (Wang, 2015). Hence, it remains a challenge to determine the required conditions associated with direct transmission even in simple alloy systems. A recent review (Wang et al., 2017) suggests that the slip transmissibility resulting from the geometric relations between incoming and outgoing slip systems significantly affects the dislocation behaviour. In the present study, we confine ourselves to studying the direct slip transmission between $a_1$ (HCP) and $b_1$ (BCC) slip systems in Ti-6242 alloy, such that the crystallographic orientation relationship is fixed and determined by the Burger Orientation Relationship (BOR), providing at least some simplification.

The present work aims to investigate dislocation transmission through $\alpha/\beta$ phase boundaries in Ti-6242 alloy, and hence address the role of dual phase morphology in its rate dependent deformation behaviour, by integrating micro-pillar test results, crystal
plasticity and discrete dislocation plasticity modelling. Section 2 gives an overview of the rate and length-scale dependent CP and the newly-developed 2D-DDP models incorporating thermally-activated dislocation escape, slip transfer and the new superposition method by O’Day and Curtin (2005). The establishment of the rate-sensitive DDP representation of the independent α and β phases in alloy Ti-6242 is given in Section 3. The α/β phase boundary barrier for slip penetration is determined phenomenologically in Section 4 using the DDP model in conjunction with corresponding crystal plasticity and experimental micro-pillar compression testing. Finally, Section 5 presents a more detailed analysis of the competition between direct and indirect dislocation transmission using a single Frank-Read source DDP model and assesses the effect of phase morphology on the rate sensitivity of titanium alloys.

2. Methodology

In this work, near-α Ti-6242 alloy (volume percentage of α phase about 90% (Qiu et al., 2014) at 293 K) is considered, which is identical to that studied experimentally using micro-pillar tests by Jun et al. (2016) and the subsequent CP modelling work by Zhang et al. (2016). In the aforementioned CP study, both the titanium alloy bases and the epoxy substrate beneath the micro-pillars were explicitly modelled to capture the accurate elastic and plastic response of the pillar material from the experimental measurements. The same constitutive laws and the extracted intrinsic properties of the α-β phases of Ti-6242 alloy are implemented in the present study, while only the pillar region is modelled explicitly to reduce the computational cost. The geometry of the micro-pillar and the α-β morphology are explicitly represented. A 2D-DDP geometric model has been established to realise a cross-section of the micro-pillar. Thermally activated dislocation escape and direct dislocation transmission are incorporated and the superposition method described in ref (O’Day and Curtin, 2005), is utilised to capture the elastic inhomogeneity of the α and β phases. The detailed formulations of these CP and DDP models respectively have been described in earlier papers (CP: (Dunne et al., 2007; Zhang et al., 2016; Zheng et al., 2016b), DDP: (O’Day and Curtin, 2005; Zheng et al., 2016c, 2017b)), hence are only concisely covered here.

2.1. Crystal plasticity finite element formulation

The CP implementation adopted is rate and length-scale dependent (Dunne et al., 2007). The total deformation gradient is assumed to be decomposed into elastic and plastic parts as

\[ F = F^e F^p \]  

(1)

in which the plastic deformation originates from crystallographic slip on defined HCP (α phase) and BCC (β phase) slip systems. The plastic velocity gradient may be expressed as

\[ L^p = \sum_i \dot{\gamma}^i n^i \otimes s^i \]  

(2)

where \( n^i \) and \( s^i \) are the slip plane normal and slip direction of slip system \( i \) respectively. The plastic shear strain rate \( \dot{\gamma}^i \) on each slip system is governed by

\[ \dot{\gamma}^i = \rho_m (b^i)^2 \nu_D \exp \left(-\frac{\Delta F^i}{kT}\right) \sinh \left(\frac{(\tau^i - \tau_c^i)\Delta V_{CP}}{kT}\right) \]  

(3)

in which \( b^i \) is the Burgers vector magnitude, \( \rho_m \) the mobile dislocation density, \( \nu_D \) the Debye frequency, \( k \) the Boltzmann constant, \( T \) the temperature, \( \tau^i \) and \( \tau_c^i \) are the resolved shear stress and the corresponding critical resolved shear stress (CRSS) on the slip system \( i \) respectively. The two rate controlling properties are the activation energy \( \Delta F^i \) and activation volume \( \Delta V_{CP}^i \). The remarkable differences of the rate sensitivity between α-basal, α-prismatic (and β phase) slip systems, and the rate sensitivity related properties \( \Delta F^i \) and \( \Delta V_{CP}^i \) are assessed and determined separately in ref. (Zhang et al., 2016).

2.2. Two-dimensional discrete dislocation plasticity formulation

In order to account for the inhomogeneous microstructures resulting from the differing properties of α and β phases in titanium alloys, a recent superposition technique (O’Day and Curtin, 2005) is utilised. The DDP boundary value problem can be solved as the superposition of several discrete dislocation (DD) sub-problems and a global fully elastic (FE) sub-problem, as schematically illustrated in Fig. 3a. The specific boundary conditions, i.e. \( u_i \) on \( S_a \) and \( T_i \) on \( S_e \), are applied to the global elastic problem and since this is dislocation-free, it can be solved using the finite element method. Each DD sub-problem is subjected to generic boundary conditions and can be solved using the classical DDP superposition method as introduced by Van der Giessen and Needleman (1995). The generic boundary conditions are chosen to be \( u_{DD} = 0 \) on \( S_a \) and \( T_{DD} = 0 \) on \( S_e \) and in addition \( u_{DD} = 0 \) is applied on the α/β phase interface between each DD sub-problem in order to retain consistency of the displacement on the shared boundary when it is solved within each neighbouring sub-problem. The local elastic part of each DD sub-problem is used to solve the generic boundary value problem and the dislocation field can be calculated assuming an infinite matrix material because each DD sub-problem is elastically homogeneous as shown in Fig. 3b.

The Peach-Koehler force acting on each dislocation can be calculated as

\[ f^{PK} = n_i (\tilde{\sigma}_i + \bar{\sigma}_i + \sigma_i^{FE}) b_i^p \]  

(4)

where \( \tilde{\sigma}_i \), \( \bar{\sigma}_i \) and \( \sigma_i^{FE} \) are the stress fields of the local elastic problem, local dislocation problem and global FE problem respectively.
In dual phase titanium alloys, a Burgers Orientation Relationship must be satisfied between the α-phase (HCP) and the adjacent β-phase (BCC) as shown in Fig. 4 (Britton et al., 2015). The BOR can be described as one closest packed plane shared by both phases, i.e. the (0001) plane in the α-phase is parallel to the (101) plane in the β-phase. In addition, one close packed direction is shared by two phases and they are indicated as the a1 and b1 directions respectively, i.e. a1//b1. Interestingly, if the two phase crystal is subjected to loading with direction parallel to the common plane, the two phases maintain plane strain conditions during deformation which is a necessary condition for a two-dimensional model. As schematically described in Fig. 5, when the loading direction is parallel to (0001)α and (101)β planes, three α-prismatic slip systems in the α-phase are potentially activated with an angle of 60° between each system, and three slip systems in the β-phase are considered which maintain plane strain as demonstrated by Rice (1987).

The model is dislocation free initially but with Frank-Read sources and obstacles randomly distributed on each slip system as shown in Fig. 5c and d. Edge dislocation dipoles can be nucleated from the sources if the stress is higher than the source strength $\tau_{\text{nuc}}$ which is generated from a normal distribution with mean value of $\tau_{\text{nuc}}$ and a standard deviation of 0.2$\tau_{\text{nuc}}$. The free flight velocity of dislocations travelling between obstacles is governed by the linear mobility law as

$$v_f = \frac{f_{\text{PK}}}{B}$$

in which $B$ is the drag coefficient. Pinned dislocations at obstacles can escape through thermal activation processes if the pinned time exceeds the critical time $t_{\text{obs}}$ = $1/\Gamma$ where $\Gamma$ is the stress related to a successful jump frequency given by

$$\Gamma = \frac{\nu_0 \beta}{l_{\text{obs}}} \exp \left( -\frac{\Delta F}{kT} \right) \sinh \left( \frac{\tau_{\text{nuc}} \Delta V_{\text{DD}}}{kT} \right)$$

in which $\nu_0$ is the Debye frequency, $l_{\text{obs}}$ the average obstacle spacing, thus the term $\nu_0 \beta/l_{\text{obs}}$ is the frequency of attempts of
Fig. 4. Schematic diagram of the Burgers Orientation Relationship (BOR) (Britton et al., 2015). The (0001) plane of alpha (HCP) phase in (a) is parallel to the (101) plane of beta (BCC) phase in (b). (c) The quantitative representation of the slip systems in $\alpha/\beta$ interphase in titanium alloys.

Fig. 5. Slip systems in the two-dimensional DDP model: (a/c) HCP crystal and (b/d) BCC crystal.
dislocations to jump the energy barrier. Dislocations may also become trapped by phase boundaries, but transmission through such a boundary is also possible if the stress on the dislocation $\tau_{\text{dis}}$ exceeds a threshold value $\tau_{\text{pass}}$. The critical value $\tau_{\text{pass}}$ for a grain boundary is a function of the misorientation between the two neighbouring grains (Li et al., 2009; Zheng et al., 2017b). However, the crystal orientation constraint from the BOR for the $\alpha$/$\beta$ interface results in only a single misorientation between $\alpha$ and $\beta$ phase slip directions, hence dislocation transmission occurs through a phase boundary if $\tau_{\text{dis}} \geq \tau_{\text{pass}}$. The determination of the threshold value $\tau_{\text{pass}}$ is addressed in Section 4.

Due to the different Burgers vector magnitude in the $\alpha$ and $\beta$ phase, a residual Burgers vector is left at the interface as a result of dislocation transmission as shown in Fig. 6. The magnitude of the residual Burgers vector is given by

$$\Delta b = N(b^\alpha - b^\beta)$$

in which $N$ is the number of dislocations transmitted across the $\alpha$/$\beta$ phase boundaries. If $\Delta b \geq b^\beta$, dislocation re-emission occurs, i.e. a new $b_1$ dislocation is generated from the residual dislocation while the residual Burgers vector becomes $-\Delta b - b^\beta$.

The material properties and modelling parameters in the crystal plasticity and discrete dislocation plasticity models are listed in Table 1, in which the properties for Ti-6242 $\alpha$ and $\beta$ phases in the CP model are those reported by Zhang et al. (2016) while those associated with the DDP model are determined here by calibration against CP model single crystal micro-pillar compression responses which in turn were obtained from the micro-pillar experiments, as discussed in the next section.

3. Strain rate sensitivity in dual phase systems

It is noted that the terms inside the ‘$\sinh$’ function in equations (3) and (6) are different for the two CP and DDP constitutive laws respectively. This is due to the differences in the mechanistic formulations: in the former, slip on each slip system occurs if the resolved shear stress $\tau$ exceeds the intrinsic slip strength together with the effects of any back stress development given by $\tau^c$ for a given slip system within the crystal plasticity model; in the latter, dislocations are explicitly represented in the DDP formulation such that the onset of slip is controlled directly by intrinsic mobility, and by back stresses established by neighbouring obstacles and dislocations which develop naturally in the DDP approach. Ensuring the same work done during the thermal activation process in both formulations thereby relates the activation volumes for the DDP approach with that for the CP model such that $(\tau - \tau^c)\Delta V_{\text{CP}} \approx \tau_{\text{net}} \Delta V_{\text{DDP}}$, in which $\tau_{\text{net}}$ is the average net stress acting on the pinned dislocations at the obstacles, and $\tau - \tau^c$ is the net driving stress for slip in CP.

From the micro-pillar compression tests (Jun et al., 2016; Zhang et al., 2016), remarkable differences in strain rate sensitivity of the differing slip system have been observed in the Ti-6242 alloy. A single crystal DDP and CP model with the dimensions $2\mu m \times 6\mu m$ (thickness for CP model is $0.2\mu m$) is set up subjected to uniaxial compression along the $y$-direction at three different constant strain...
rates up to 4% strain. The crystal orientations with respect to the loading direction are shown in the sub-figures in Fig. 7. The orientations are chosen such that only the slip system of interest is the most favourable to be activated, i.e. α-prismatic in Fig. 7a, α-basal in Fig. 7b and β-(121)[111] in Fig. 7c. The strain rates are chosen for which a strong positive strain rate sensitivity is known to occur. The identical activation energies $\Delta F$ are argued to be relevant and hence used for both DDP and CP models, as reported in ref (Zhang et al., 2016). while the source strength $\tau_{nuc}$ and activation volume $\Delta V_{DD}$ are determined by calibration against the stress-strain responses. The energy balance above is then utilised to validate the corresponding activation volume, $\Delta V_{DD}$. All remaining DDP model parameters (e.g. mobility coefficient and nucleation time) are as reported by Zheng et al. (2017a). In summary, the experimental micro-pillar tests provide for the determination of the CP model properties which in turn facilitates the determination of the remaining DDP properties by ensuring the DDP model gives the same response as that for the CP model. The resulting stress responses at different strain rates for the CP and DDP models are shown in Fig. 7 and the Ti-6242 properties are summarized in Table 1. Full details of the original CP model comparisons with experimental micro-pillar tests may be found in (Jun et al., 2016; Zhang et al., 2016).

Strong positive strain rate sensitivity is observed for both α and β phases over the strain rate range $10^{-5}$ to $10^{-2}$s$^{-1}$. The strain rate sensitivities of each slip system in the orientations shown in Fig. 8 are summarized in Fig. 8 in log-log form in which the slope of the curve represents the strain rate sensitivity (SRS) $m$ as

\[ m = \frac{d\log \varepsilon}{d\log \dot{\varepsilon}} \tag{8} \]

The SRS (the gradient of the graphs given in Fig. 8) for all slip systems can be seen to vary with strain rate, shown increasing for the range considered. Between $10^{-5}$ to $10^{-3}$s$^{-1}$, the SRSs $m$ for the β phase and α-basal are not dissimilar (0.16 and 0.17 respectively) and are higher than that for α-prismatic $m = 0.04$ at strain rate in excess of about $10^{-2}$s$^{-1}$. The significant anisotropy of the rate dependence of single crystal titanium slip leads to the microstructural and textural dependence of the overall polycrystal strain rate.
sensitivity. The strain rate sensitivity of each slip system is an intrinsic property but the overall polycrystal rate dependence varies significantly with microstructure and external loading conditions. For instance, alpha titanium alloys display different strain rate sensitivity with respect to different HCP textures, and the α-variants in basket weave structures in dual phase titanium alloy also lead to significant effect on the overall SRS (Zhang and Dunne, 2017).

4. Determination of the critical stress associated with dislocation transmission across α/β phase boundaries

Fig. 2a shows the experimentally observed slip development (Zhang et al., 2016) in a given α-β Ti-6242 micro-pillar at the end of uniaxial loading. The transient analysis of the slip development facilitated the determination of the point in the loading history at which slip (on the sample free surface) was first observed to initiate in the β phase. In parallel, the CP modelling (also shown in Fig. 2a) provided reasonable quantitative assurance that the important features of the slip nucleation, localisation and penetration into the β phase were captured accurately, along with the quantitative rate-sensitive stress-strain response (Fig. 2b). Hence, the approach adopted to estimate the DDP criterion for slip transmission across the α–β interface is to carry out direct comparison between CP and DDP analyses of an identical α+β micro-pillar for which the CP results show close agreement with the experiment, and for which a pillar cross-section can be found for which plane strain conditions hold.

Such a micro-pillar is shown in Fig. 9a. The mid-cross section shown in Fig. 9b is modelled using DDP since it satisfies the plane strain condition when the pillar is subjected to uniaxial compression along the y-direction. An average strain rate of $2 \times 10^{-5}$ s$^{-1}$ is applied on the top surface up to 0.02 strain and the $a_1$ and $b_1$ slip systems are potentially activated. Due to the tapered geometry of the pillar and the low critical resolved shear stress of the α-prismatic system well-orientated for slip, plasticity is first generated in the α phase around the corners on the top surface of the micro-pillar. The effective plastic strain $p$ in the fully 3D CP micro-pillar model is monitored during the loading history, where $p$ is given by

$$p = \left(\frac{2}{3} \varepsilon_p : \varepsilon_p\right)^{1/2}$$

in which $\varepsilon_p$ is the plastic strain tensor. Fig. 10 shows the CP effective plastic strain distributions along path B-B', given in Fig. 9b, which are extracted at two instances during the pillar loading history. At $t = 4.40$ s in the loading, slip develops in the α phase and peaks at the α/β interface, but the β phase remains elastic at this instant. With further loading, at $t = 4.96$ s, the plasticity in the α phase has increased and importantly, the first occurrence of slip is found to occur in the β phase. The slip distribution so obtained is from the CP micro-pillar model; because this model does not explicitly account for dislocations, it is not feasible to determine if the β slip has arisen from dislocation transmission from α to β phase, or whether new dislocations have been nucleated in the β phase as a result of the stress state established by slip in the adjacent α phase. However, the DDP model does explicitly represent dislocations and can differentiate between dislocation transmission and new dislocation nucleation. For this purpose, the DDP model results for the same micro-pillar are now compared directly with the CP results just before and after the slip becomes apparent in the β phase from the CP model.
Firstly, the effective elastic strains $q$ due to dislocations and their interactions from the DDP analysis, defined by

$$q = \left( \frac{2}{3} \bar{\varepsilon} : \bar{\varepsilon} \right)^{1/2}$$

are shown for $t = 4.40s$ and $t = 4.96s$ in Fig. 11, together with the CP-calculated plastic strain fields. At $t = 4.40s$, Fig. 11a and c shows there is no plasticity in the $\beta$ lath according to the CP model, and the DDP model similarly shows no dislocation content (and hence no elastic strain field) within the $\beta$ phase, but significant plastic deformation occurs within the $\alpha$ phase in both models. Multiple discrete $\alpha$ prismatic slip bands are formed in the DDP model compared to the rather homogeneous plastic zones in the CP model reflecting the differing ways in which plasticity is modelled by the two techniques.

Before considering further the DDP modelling results at the second loading instance of $t = 4.96s$, for which the CP model shows the first development of slip in the $\beta$ phase lath (Figs. 10 and 11b), it is necessary to assess the DDP criterion for local slip transmission across the $\alpha - \beta$
interface versus β-phase dislocation nucleation. Dislocation transmission is taken to be driven by the local resolved shear stress acting on the dislocation at the interface; if the resolved shear stress exceeds a critical stress, $\tau_{\alpha\beta}$, then dislocation transmission is allowed. Otherwise (i.e. resolved shear stress $< \tau_{\alpha\beta}$), dislocation transmission is prohibited. Hence if the critical resolved shear stress for dislocation transmission is taken to be infinite in the DDP model (i.e. direct slip transmission is prohibited), we find that the DDP model does not show dislocation nucleation within the β phase such that the CP model predictions of experimentally-observed micro-pillar β-phase slip development are not reproduced at the loading instance of $t = 4.96s$. Hence, in order to reproduce the CP and experimental observations of β slip development at this loading instance, it was necessary to allow for direct dislocation transmission within the DDP model with a critical shear stress of $\tau_{\alpha\beta} = 5430$MPa. But note that allowing for slip nucleation alone (by inhibiting direct dislocation transmission by choosing $\tau_{\alpha\beta} = +\infty$) was not

![Fig. 11. (a/b) Effective plastic strain contours in crystal plasticity model; (c/d) effective (elastic) strains due to dislocations in the discrete dislocation plasticity model. (a/c) before α−β slip transmission and (b/d) after α−β slip transmission. (e) Local SEM image on the free surface of the micro-pillar after compression (Zhang et al., 2016). Multiple slip bands are developed in the β phase which are parallel to the $a_1$ slip bands in the α phase.](image-url)
found to give rise to $\beta$ slip, hence it is argued that dislocation transmission is essential to explain the observations. Other authors have pointed out that slip transmission is also heavily dependent on the atomistic structure and geometric orientation of the interfaces (Wang, 2015), hence the critical shear stress determined here is appropriate for the specific crystallographic and geometric combination shown in Fig. 9, but the methodology can be generalised to other circumstances. With this critical shear stress for direct slip transmission, the corresponding DDP results for the effective (elastic) strain field are shown in Fig. 11d. Here, dislocations transmit to the $\beta$ phase establishing the elastic strain field shown, indicating the establishment of slip in the $\beta$ phase and showing good agreement with the CP observations in Figs. 10 and 11b. In addition, from the local SEM image of the compressed micro-pillar, multiple slip bands were observed in the $\beta$ phase which are parallel to the $b_1$ slip bands in Fig. 11d. Hence we have established the critical shear strength of the $\alpha-\beta$ interface in the alloy Ti-6242. Further, because of its quantification within the DDP framework, it becomes possible to investigate the conditions necessary to drive indirect slip transmission, that is, the nucleation of new dislocations within the $\beta$ phase as a result of the stress states established by slip pile-up at the $\alpha-\beta$ interface, versus those which lead to direct dislocation transmission and hence direct slip transfer. This is investigated further in Section 5, but finally here, Fig. 12 shows the comparison of the DDP total (effective) strain versus the effective strain field obtained from the CP model at an applied average strain of 1%. The strain fields are very similar except that of course the DDP model captures much more of the slip localisation remaining in the lower part of the $\alpha$ crystal resulting from the $a$ prismatic slip. In order to quantitatively compare the total strain distributions, 100 vertical paths which are parallel to B-B’ falling within the middle third of the pillar are utilised to determine the averaged strain distribution shown in Fig. 13. The results of the CP and DDP models show good agreement when the much more discrete DDP analysis is averaged.

![Fig. 12. Effective strain distribution at 1% strain from (a) DDP and (b) CP modelling.](image)

![Fig. 13. Comparison between DDP and CP predicted effective strain distributions.](image)
5. Discrete dislocation plasticity analysis of the competition between direct and indirect dislocation transmission

Some important general questions remain about slip transmission, including how often does direct slip transfer occur, is it the predominant mechanism even when sources in front of pile-ups are active, or is it in fact much more likely to observe indirect transmission due to the stresses generated by pile-ups adjacent to the boundary of interest? In order to address these questions, a much simpler single source DDP model is used, shown schematically in Fig. 14. The crystal is dislocation-free initially but a Frank-Read source is located at the left-bottom corner of the model and its slip plane is oriented $45^\circ$ with respect to the positive $x$-axis. The slip plane is terminated at the specified length $d_{obs}$ from the source and the termination can be treated as either an obstacle or a grain boundary; for the former, thermal activation may facilitate dislocation escape from the obstacle but for the latter, the grain boundary is modelled as impenetrable. Single pile-up can be formed when the model is subjected to uniaxial tension along the $y$-axis such that the other half of each dipole escapes from the left free surface. A constant stress $\tau_{app} = \tau_{nuc} + 100\text{MPa}$ is applied on the top surface and the results are extracted when all dislocations reach equilibrium. The same model is utilised for three sets of crystal properties: $\alpha$-basal, $\alpha$-prismatic and $\beta$ phase. For a given source strength, the number of dislocations in the pile-up as well as the stress on the leading dislocation is a function of the slip plane length $d_{obs}$.

Fig. 15 shows the results of the three different crystal structures with slip plane length $d_{obs}$ varying from $0.2\mu m$ to $0.8\mu m$ for the case where the slip plane terminates at an obstacle. The first observation in Fig. 15a is that the number of dislocation in the pile-up increases with increasing slip plane length. As a result, the stress acting on the leading dislocation also increases as shown in Fig. 15b. The rate of increase in the number of dislocations for the case of BCC $\beta$ slip is higher compared to $\alpha$ prism and basal slip due to its lower modulus and smaller Burgers vector which results in a lower back stress for each dislocation. When the pile-up is formed in

![Fig. 15. Schematic representation of single source DDP model.](Z. Zheng et al. International Journal of Plasticity 104 (2018) 23–38)
front of an obstacle, the leading dislocation experiences a thermal activation process which potentially enables it to escape the obstacle and continue to glide. The SRS at low strain rates, e.g. \( \dot{\varepsilon} \leq 10^{-5}\text{s}^{-1} \) is controlled by the time constant associated with thermally activated escape \( t_{obs} \) (Zheng et al., 2016c). Fig. 15c relates the time constant to the obstacle-source spacing for the three crystal structures. In general, the escape time decreases with increasing pile-up size due to the increasing stress on the leading dislocation. On the other hand, the time constant is also a function of the intrinsic properties of the slip systems such as activation energy and volume. Hence, the time constant, or the strain rate sensitivity of the \( \alpha \)-prismatic system is found to be more sensitive to the change in the average obstacle-source spacing as demonstrated in Fig. 15c.

When the termination of the slip plane in Fig. 14 is a phase boundary, i.e. the single pile-up is formed at an interface, the stress on the leading dislocation may assist in transferring it to the adjacent grain. By comparing the stress developed by the \( \alpha \)-prismatic pile-up to the critical stress \( \tau_{eff} \) determined above for \( \alpha/\beta \) dislocation transmission in Fig. 15b, under the given loading conditions, the trapped \( \alpha \) dislocation at the grain boundary is able to transfer to the \( \beta \) phase when the length of the pile up is longer than 0.6\( \mu \)m. However, the figure shows that the nucleation of \( b_1 \) dipoles may happen much earlier, long before the stress on the leading \( \alpha \) dislocation becomes high enough to drive direct slip transmission, indicating in this scenario that indirect slip transmission at the \( \alpha/\beta \) interface is greatly preferred. In fact, if a \( b_1 \) dipole is nucleated due to the stress concentration from \( \alpha \) pile-ups, the stress on the pile-ups is relaxed due to the opposite pile-up formed at the phase boundary in the \( \beta \) phase. Fig. 16 shows the resolved shear stress distribution of the \( b_1 \) slip system in front of an \( \alpha \) prismatic pile-up within the dotted box indicated in Fig. 14. The colour map is chosen such that the grey colour represents a shear stress that is higher than the average source strength in the \( \beta \) phase. Two different boundary-to-source spacings are considered, namely \( d_{obs} = 0.4\mu \)m and 0.8\( \mu \)m. When the length of the pile-up is 0.4\( \mu \)m, the stress on the leading dislocation is not high enough to drive the transmission but as shown in Fig. 16a, if there are sources located in the grey region, \( b_1 \) dipoles can be generated hence indirect slip transmission occurs. On the other hand, if the distance from the source to the boundary is 0.8\( \mu \)m which is higher than the critical distance of dislocation transmission, direct slip transfer is possible. However, as shown in Fig. 16b, the stress concentration area is also larger compared to the small pile-up case. Here the grey region is divided into two parts: part A (hatched) is the stress concentration region within which the stress on the leading dislocation just reaches the transmission stress \( \tau_{eff} \), and part B is the unmarked grey region within which the stress increase results from the dislocation structure reaching equilibrium. There are three different scenarios with respect to direct and indirect slip transfer competition: (1) There is no source in either region A or B, slip transfer is possible but is purely direct transmission dominated. (2) There are sources located in region B but no source in region A, and even though the sources are located in a high stress area, direct dislocation transmission occurs before the stress on the sources exceeds their strength; and with dislocation transmission, the stress in front of the pile-up drops and the process repeats. This scenario is also therefore dominated by direct slip transfer. (3) There are sources in region A, and nucleation of new dipoles occurs before the leading dislocation transmits, followed by a corresponding stress drop on that dislocation so that direct transmission may not be activated. To summarise, direct slip transfer can only occur if the size of the pile-up is large enough to drive the transmission event and the material in front of the pile up is source-free to restrain the nucleation of new dipoles.

As discussed earlier, the strain rate sensitivity, or equivalently, the time constant associated with dislocation escape from obstacles, depends on the size of the pile-up. It has also been reported that the \( \beta \) volume fraction and \( \alpha/\beta \) morphology have significant effects on the SRS in titanium alloys (Zhang and Dunne, 2017). Here we use the single source model to investigate the effect of \( \beta \) laths on the overall SRS schematically. If we consider a single \( \alpha \) slip plane with one source and obstacle as shown in Fig. 17a, one pile-up group is formed in front of the obstacle under the external shear stress. The time of thermally activated dislocation escape is determined by the size of the pile-up which is controlled by the source-obstacle spacing and the magnitude of the external stress. If a thin \( \beta \) lath is located between the source and the obstacle as shown in Fig. 17b, two separate pile ups are formed due to the impediment to slip from the phase boundary. The resulting average pile-up size is smaller compared to the case of pure \( \alpha \) phase (in the absence of a \( \beta \) lath) hence the time constant increases due to the decrease of the stress on the pinned dislocation. For more complex situations where the \( \beta \) lath is thick as shown in Fig. 17c, or multiple thin \( \beta \) laths exist as shown in Fig. 17d, the single pile up is divided into several small pile-up groups. The \( \beta \) volume fraction in these two cases is larger and the time of escape is longer.
An important example for which the above explanation is important is in the differing cold creep response, and hence dwell fatigue susceptibility, of the Ti-6242 and Ti-6246 alloys. The microstructural characterisations by Qiu et al. (2014) have revealed that the volume fraction of β phase in Ti-6246 is higher (∼40% as opposed to ∼10% in Ti-6242) and the average α grain size is smaller (5.3μm as opposed to 13.6μm in Ti-6242). From the analysis in the present study, the time constant associated with Ti-6246 microstructures (Fig. 17d) is hence larger compared to the Ti-6242 microstructure (Fig. 17a/b), hence leading to the very different creep responses in the two alloys. Previous work by Zheng et al. (2016a) in which the homogenised α-β behaviour was studied using DDP also demonstrated that thermally activated dislocation escape in a Ti-6246 alloy microstructure was more difficult compared to a Ti-6242 microstructure resulting in a lower average dislocation velocity in the former alloy, reflecting its lower cold creep rate than for the Ti-6242 microstructure.

### 6. Conclusion

Integrated experimental micro-pillar compression testing, crystal plasticity and discrete dislocation modelling of two-phase alloy Ti-6242 have been utilised to investigate slip transfer at α-β interfaces and its influence on strain rate sensitivity and hence cold creep with the following conclusions.

1. Strain rate sensitivities of α-basal, α-prismatic and β-(12T)[11T] slip systems in Ti-6242 alloy have been investigated. The SRSs of β slip and α-basal slip are similar to each other and higher than that for α-prism slip for strain rates between $10^{-3}$ to $10^{-5}$ s$^{-1}$.
2. The critical stress associated with dislocation transmission across an α/β phase boundary has been determined to be 5430MPa by direct comparison of DDP and CP micro-pillar compression results with independent experimental results. Crystal plasticity modelling is demonstrated to be able to capture both overall stress response and local plastic strain development even without explicit representation of dislocation transmission across α/β interfaces in a two-phase micro-pillar.
3. A single Frank-Read source DDP model is established in order to study the competition between direct dislocation transmission and the indirect slip transfer which results from the nucleation of sources in front of pile-ups. Direct slip transfer can only occur if the size of pile-ups is large enough to drive the transmission event and the material in front of the pile-up is source-free to restrain the indirect transfer, otherwise slip transfer is dominated by indirect transmission.
4. The strain rate sensitivity of dual phase titanium alloys is strongly affected by the α/β morphology. The average size of pile-ups reduces with the presence of β laths, hence the time constant of thermal activation events increases which results in differing overall SRS.

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Fig. 17. Schematic diagram showing the effect of β laths on the size of pile ups: (a) pure α phase; (b) single thin β lath; (c) single thick β lath and (d) two thin β laths.
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