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Investigation of slip transfer across HCP grain boundaries with application to cold dwell facet fatigue

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ABSTRACT

This paper addresses the role of grain boundary slip transfer and thermally-activated discrete dislocation plasticity in the redistribution of grain boundary stresses during cold dwell fatigue in titanium alloys. Atomistic simulations have been utilised to calculate the grain boundary energies for titanium with respect to the misorientation angles. The grain boundary energies are utilised within a thermally-activated discrete dislocation plasticity model incorporating slip transfer controlled by energetic and grain boundary geometrical criteria. The model predicts the grain size effect on the flow strength in Ti alloys. Cold dwell fatigue behaviour in Ti-6242 alloy is investigated and it is shown that significant stress redistribution from soft to hard grains occurs during the stress dwell, which is observed both for grain boundaries for which slip transfer is permitted and inhibited. However, the grain boundary slip penetration is shown to lead to significantly higher hard-grain basal stresses near the grain boundary after dwell, thus exacerbating the load shedding stress compared to an impenetrable grain boundary. The key property controlling the dwell fatigue response is argued to remain the time constant associated with the thermal activation process for dislocation escape, but the slip penetrability is also important and exacerbates the load shedding. The inclusion of a macrozone does not significantly change the conclusions but does potentially lead to the possibility of a larger initial facet.

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1. Introduction

Cold dwell fatigue continues to be a serious industrial concern since it was first detected in titanium discs in aero-engines in the early 1970s [1,2]. A significant lifetime reduction, known as dwell life debit, is known to occur when some Ti alloys are subjected to fatigue loading that includes a stress hold period at the maximum stress magnitude, i.e. a dwell period [1,3], during each loading cycle. There is considerable evidence demonstrating that cold dwell fatigue is associated with the formation of facet cracks [4] on hexagonal close packed (HCP) basal planes orientated within about ±15° to the normal to the primary loading direction [1,5]. The combination of a well-oriented (soft) grain adjacent to a badly-oriented (hard) grain is argued to be important for facet crack nucleation [6–8]. Stroh [9] established that a dislocation pile-up terminating at a grain boundary leads to high stress in the adjacent grain that might be sufficient to nucleate a crack. Stroh’s model supports the necessity of a hard-soft crystallographic orientation combination to nucleate a facet crack [1], but does not address the role of the dwell period (or equivalently, the material rate-dependence), nor the effect of the penetrability of the grain boundaries (GBs) for slip transmission. Hasija et al. [10] were the first to explain the load shedding phenomenon by showing the stress redistribution from the soft grain to the hard grain during the stress hold period. The strong rate sensitivity of titanium alloys at low temperature (e.g. 20 °C) has recently been studied in some detail and has been quantified at the single-crystal level [11–13] and at the macro-level [3], and is argued to be mechanically fundamental to cold dwell fatigue [14,15]. The temperature-dependent creep and load shedding behaviour of near-α Ti alloys was recently examined by Zhang et al. [16] using crystal plasticity modelling, who showed that the dwell debit depends crucially on temperature; the worst case dwell debit occurred at 120 °C in the alloy considered.

The remarkably differing dwell fatigue responses of the two alloys, Ti-6242 and Ti-6246, have been studied by Zheng et al. [17] using an integrated crystal plasticity and discrete dislocation...
plasticity (DDP) approach. They first utilise crystal plasticity modelling to extract the thermal activation energies for pinned dislocation escape for the two alloys based on independent experimental data [3]. Then they utilise a recently developed thermally-activated discrete dislocation plasticity model [18] to examine the stress distribution within the soft-hard grain combinations under dwell fatigue loading. The energy barrier for dislocation escape for alloy Ti-6242 was found to be lower than that for Ti-6246, but interestingly the macroscopic rate sensitivities of the two alloys under displacement-controlled loading, over the range of strain rates considered, are found to be very similar. However, under stress dwell loading conditions, remarkable stress redistribution from the soft grain to the basal plane normal stresses in the hard grain was observed in alloy Ti-6242, whereas Ti-6246 showed negligible load shedding as a consequence of its higher thermal activation energy. The study by Zheng et al. [17] provides a mechanistic explanation of the dwell debit differences arising in alloys Ti-6242 and Ti-6246, and explains the dwell sensitivity of titanium alloys. However, the assumption of impenetrable grain boundaries used in the DDP modelling in their study might influence the stress concentration at the soft-hard grain boundary in dwell and/or the level of slip activation in the adjacent hard grain. In particular, the peak stress increase resulting from load shedding during the stress dwell period could depend upon the inhibition or otherwise of slip transfer at the hard-soft grain boundary, hence the role of dislocation pinning, transmission and residue at grain boundaries is potentially important.

Grain boundaries play a crucial role in the plastic behaviour of polycrystalline materials. The Hall-Petch [20,21] equation relates the material strength, e.g. yield stress $\tau_y$, to the grain size $d$ as

$$\tau_y = \tau_0 + K d^{-0.5}$$

where $\tau_0$ can be identified as the single-crystal or large-grain limit, and $K$ is a material constant representing the contribution to the yield stress from grain boundaries. The grain boundaries enhance the material strength by hindering the extension of slip across the material. Dislocation transfer through a GB can be due to indirect or direct transmission as illustrated in Fig. 1(a) and (b) respectively. Indirect transmission mainly results from the nucleation of Frank-Read sources located in the stress concentration area, e.g. in front of a dislocation pile-up [22]. On the other hand, if the stress acting on the leading dislocation of a pile-up is high enough, that leading dislocation might be able to directly transfer to a new slip plane, which normally has low misorientation angle with respect to the originating plane, accompanied by the formation of a residual dislocation at the grain boundary to conserve the overall Burgers vector. Lee et al. [23] propose three conditions governing direct slip transmission through grain boundaries: the (I) geometric condition, (II) resolved shear stress condition and (III) residual grain boundary dislocation energy minimization condition. Experimentally, Wang et al. [24] and Simkin et al. [25] characterised slip transfer in the activation of deformation twinning at grain boundaries. Britton et al. [26] carried out nanoindentation tests on cubic materials and found that the grain boundary with greater misalignment of slip systems tended to exhibit higher resistance to slip transfer. In modelling approaches, Liu et al. [27] found using 3D dislocation dynamics simulations that grain boundaries can strongly obstruct dislocation transmission even at low misalignment. Dunne et al. [7] and Zheng et al. [28] have demonstrated that ‘indirect slip transfer’ occurs in dwell fatigue from prismatic systems in the soft grain to the adjacent basal systems in the hard grain by utilising crystal plasticity and discrete dislocation plasticity respectively, and also observed that the slip development is grain boundary morphology dependent. The analysis of slip transfer in terms of the geometrical alignment of activated slip systems in neighbouring grains using both experiment and modelling techniques have recently been reviewed by Bieler et al. [29]. The static grain boundary energies as a function of the misorientation between neighbouring grains were calculated by several authors utilising well-developed atomistic simulations in both cubic [30–33] and hexagonal close-packed materials [34–37]. The energy barriers to dislocation transmission across individual GBs were quantified by Sangid et al. [38]. An inverse relationship between the energy barrier for dislocations to penetrate a GB and the static energy was developed from their analysis to be

$$E_{\text{Barrier}} = 2.8 \times 10^{13} \cdot (E_{\text{GB}}^{\text{Static}})^{-0.6}$$

The transmission energy barrier in Ref. [38] is normalised by the volume of the simulation control box which requires extreme care to select. It is clear from Ref. [38] that the power law in equation (2) is valid only for the considered GBs in the Ni alloy studied and cannot easily be generalised to other materials. Another approach to calculating the energy barrier of dislocation transmission was established by Li et al. [39] who used 2D discrete dislocation plasticity modelling by incorporating direct slip penetration to study the Hall-Petch effect. The transmission energy criterion is there argued to be linearly related to the static grain boundary energy plus the strain energy of newly generated residual dislocations as

$$E_{\text{Barrier}} = E_{\text{GB}}^{\text{Static}} b + \alpha G (\Delta b)^2$$

where $b$ and $\Delta b$ are the magnitudes of the Burgers vectors of incoming and residual dislocations at the GB respectively. Calculation of the precise magnitude of the dislocation transmission energy barrier requires significant computational time (the

Fig. 1. Schematic diagrams showing the (a) indirect and (b) direct slip transmission through grain boundaries.
methodology is described by Sangid et al. [38]).

In this study, we first calculate HCP static grain boundary energies in terms of misorientation angles in two neighbouring grains of symmetric tilt grain boundaries (STGBs) and asymmetric tilt grain boundaries (ATGBs) of titanium alloy utilising atomistic simulations. The grain boundary orientation effect on the static GB energy is also assessed. This energy is then utilized within a discrete dislocation formulation, in which the dislocation transmission energy is the summation of a magnification of the static GB energy and the strain energy of residual dislocation left at GBs. The magnification coefficient of the static GB energy is utilized in order to reflect the difference between static GB energy and the penetration energy for dislocation transmission as discussed by Sangid et al. [38]. In addition, it then becomes possible to carry out sensitivity studies of the GB penetration energy on slip transfer. The DDP model also incorporates rate sensitivity arising from thermally-activated dislocation escape from obstacles. The size effect in polycrystalline Ti-6242 alloy at different strain rate regimes is assessed considering impenetrable and penetrable GBs. We then employ the DDP slip transfer model to investigate the load shedding between soft and hard grains in alloy Ti-6242 under dwell fatigue conditions in order to address the role of grain boundary slip transmission in dwell fatigue behaviour. The effect of grain boundary energy barrier on the behaviour of load shedding is presented. Finally, because of their perceived importance in dwell fatigue, a macrozone, or micro-textured region (MTR) is studied with the new DDP model.

2. Atomistic simulations of HCP static grain boundary energies

Static grain boundary energies are computed by minimizing the system energy of a bicrystal computational cell with 3D periodic boundary conditions using the conjugate-gradient method in the LAMMPS code [40]. Several 0 K minimum energy GB structures are obtained by utilising successive rigid body translations followed by an atom deletion technique introduced by Tschopp and McDowell [41,42]. More than 15,000 initial configurations were relaxed for each misorientation angle and the minimum GB energy was determined for the misorientation. Grain boundary energies are calculated using embedded atom method (EAM) interatomic potentials [43] which have been demonstrated to reproduce the elastic and plastic behaviour of titanium reasonably well [44].

Two types of GBs, namely STGB and ATGB, were considered as shown in Fig. 2. The grain boundary sits parallel to the x-z plane and the appropriate rotation about the z-axis, i.e. [0001] direction, is performed to achieve the desired misorientation of STGB. Similar calculations for the same tilt axis in titanium were performed by Wang et al. [35]. The comparison of this work with results of symmetrical [0001] tilt boundaries [35], together with [1T00] and [1210] misorientation axes [34,36], are shown in Fig. 3. Reasonably good agreement with established data is observed and the energies with a range of tilt axes are found to be a similar order of magnitude to that for STGBs. Furthermore, asymmetric tilt grain boundaries are also generated as shown in Fig. 2(b): the crystal orientation of the lower crystal is fixed with its c-axis parallel to the x-direction while the c-axis of the upper crystal is directed along the z-axis and rotated about [0001] direction. The same methodology for STGBs was adopted to calculate the grain boundary energies, plotted against the inclination angle $\phi^*$ in Fig. 4. The calculated ATGB energy values are found to be slightly higher than those for STGBs. Additionally, the GB energy varies strongly with the inclination angle when $\phi^*$ is close to 0° and 60° but becomes almost independent of the angle when $20^\circ \leq \phi^* \leq 40^\circ$.

In two dimensional geometries, for a particular crystallographic misorientation, the static grain boundary energy is also a function of grain boundary orientations. Two particular crystallographic misorientations $\phi = 42.1^\circ$ and $\phi^* = 30^\circ$, which give the highest boundary energy of STGB and ATGB respectively, are chosen to investigate the grain boundary orientation dependence. As shown in Fig. 5, the inclination angle with respect to the reference orientation in Fig. 2 of STGB and ATGB is indicated by $\beta$ and $\beta^*$ respectively. The calculated static grain boundary energies are summarised in Fig. 6. The grain boundary orientation is found to play a negligible effect on STGB energy while the ATGB energy is found to reduce to almost 1/3 of the reference orientation for some grain boundary orientations.

3. Discrete dislocation plasticity formulation incorporating slip transfer

A 2D discrete dislocation model with GB-dislocation penetration was first introduced by Li et al. [39] to study the Hall-Petch effect in a cubic crystal in a high strain rate regime ($\dot{\varepsilon} > 10^3 s^{-1}$). It has been argued that the main slip controlling mechanism at low strain rate ($10^{-5} s^{-1} \leq \dot{\varepsilon} \leq 10^2 s^{-1}$) in Ti alloys is that of thermal activation of pinned dislocation escape from obstacles [6,18]. A two-dimensional DDP model, which considers both dislocation transmission across grain boundaries and thermally-activated dislocation escape from obstacles, is first presented and tested against the impenetrable GB model under displacement-controlled loading in different strain rate regimes. We then utilise the DDP model to examine the dwell fatigue response of Ti-6242 alloy, in order to address the effect of grain boundary penetrability in the soft-hard grain combinations by comparing with the impenetrable model. The details of the penetrable GB and thermal activation discrete dislocation plasticity model have been described in full in earlier papers [18,39], hence are covered only briefly as follows.

![Fig. 2. Atomic representation of (a) symmetric tilt grain boundary (STGB) and (b) asymmetric tilt grain boundary (ATGB). Upper half of the crystal rotated clockwise around the [0001] direction. The misorientation angle of the STGB is $\phi$ and the inclination angle of the ATGB is $\phi^*$.](image-url)
3.1. The GB slip transfer model

Two main processes are considered in the GB slip transfer model: (I) direct transmission of dislocations across the grain boundaries and (II) dislocation re-emission from the residual dislocation content at the GBs. The geometric and residual grain boundary dislocation energy minimization conditions for slip transfer are established by considering the incoming and outgoing active slip systems at a grain boundary, and the associated resolved shear stresses. Consider a group of dislocations piling up at the GB as shown in Fig. 7(a); the resolved shear stress \( \tau \) acting on the leading dislocation must be larger than or equal to the critical value \( \tau_{\text{pass}} \) to enable the penetration of the GB, as described in Ref. [39], which may be expressed energetically as

\[
\tau b_1^2 \geq \tau_{\text{pass}} b_1^2 = \omega E_{\text{gb}} b_1 + \alpha G(\Delta b)^2
\]

in which \( b_1 \) and \( \Delta b \) are the magnitudes of the Burgers vectors of incoming and residual dislocations at the GB respectively, where \( \Delta b = b_1 - b_2 \) and \( b_2 \) is the Burgers vectors of the outgoing dislocation, \( \alpha \approx 1 \) (a material constant), \( G \) the shear modulus and \( E_{\text{gb}} \) is the GB energy per unit area. The coefficient \( \omega \) is introduced to represent the magnification of the static grain boundary energy in order to provide a representation of the penetration energy for a dislocation to transmit across the GB. Sangid et al. [38] found that the highest energy for dislocation penetration (for \( \Sigma 3 \) GBs) is about 2–4 times higher than that for the majority of other GBs. Furthermore, with the consideration of the grain boundary orientation effect, the value of \( \omega \) is chosen within the range of 0.5–4 in order to provide a sensitivity study of slip transfer in terms of GB penetration energy and grain boundary orientation. This range includes the value of \( \omega = 1 \) which corresponds to the original slip transmission DDP model presented in Ref. [39] so that the consequences of differing GB penetration (as opposed to static) GB energies may be assessed. It is made clear in subsequent sections where non-unity
values of $\omega$ are assessed. The value of $E_{GB}$ as a function of misorientation angle and grain boundary orientation is obtained from atomistic simulations as discussed earlier and shown in Figs. 3–6. The left-hand term of inequality (4) is the external work done by the shear stress $\tau$ on the leading dislocation of the pile-up. The two terms on the right of inequality (4) represent the dislocation transmission energy barrier and the strain energy of the residual dislocation.

The residual dislocation re-emission, as described in Fig. 7(b), is also considered in the model. From the energy point of view, the re-emission of the accumulated dislocation must satisfy the following condition:

$$aG(\Delta B)^2 \geq \left[ aGb^2 + aG(\delta b)^2 + \frac{Gb^2}{2\pi(1-\nu)} \sum_{i=1}^{n} \ln \left( \frac{R}{x_i} \right) \right]$$

(5)

in which $\Delta B$, $b$ and $\delta b$ are the magnitudes of Burgers vectors of accumulated residual dislocation before re-emission, the emitted dislocation and the newly generated residual dislocation respectively, and $\nu$ is the Poisson’s ratio, $R$ is the screening length of the dislocation stress field, and $x_i$ is the distance between the emitted dislocation and the $i$th dislocation on the out-going slip plane before the dislocation re-emission event. The left term of equation (5) is the energy of accumulated dislocations while the right terms denote the energy of the emitted dislocation, new residual dislocations and the elastic interaction energy between the emitted dislocation with the dislocations on the outgoing slip plane. In order to emit a complete dislocation, the projection of the accumulated dislocation magnitude $\Delta B$ on the outgoing plane must be larger than or equal to one Burgers vector magnitude.

3.2. The thermally-activated DDP model

The origin of the strain rate sensitivity of the model arises from three key mechanisms, namely dislocation nucleation from Frank-Read sources, dislocation mobility along slip planes and thermally activated dislocation escape from pinning obstacles. The rate-sensitive behaviour is predominated by nucleation and mobility of dislocations in the strain rate range $10^2$ to $10^5 s^{-1}$ while it is argued that thermal activation processes dominate when the strain rate is lower than about $10^2 s^{-1}$ [18]. Dislocations in the model are nucleated from randomly distributed Frank-Read sources if the stress $\tau$ acting on the source exceeds its strength $\tau_{nuc}$ for a period of time $t_{nuc}$. The nucleation time is estimated by Agnihotri and Van der Giessen [45] as

$$t_{nuc} = \frac{\eta \varphi}{C_0 b}$$

(6)

in which $\varphi$ is the half-length of the source segment, $b$ is the magnitude of the Burgers vector and $\eta$ is a constant related to the viscous drag coefficient $C$. The source strengths satisfy a Gaussian distribution with average $\tau_{nuc}$ and standard deviation $0.2 \tau_{nuc}$. The initial nucleation spacing $L_{nuc}$ is taken such that the attraction stress between two opposite dislocations is equilibrated by the applied stress field $\tau_{nuc}$. If two dislocations of opposite signs move together within the annihilation distance $L_p = 6b$, they are eliminated from the model. The free flight of dislocations is governed by the mobility law

$$v = \frac{\tau b}{B}$$

(7)

A cut-off velocity $v_{co} = 20 m/s$ is introduced to resolve the dislocation dynamics. Gliding dislocations may also be obstructed by randomly distributed obstacles. Pinned dislocations are released after a critical period of time which can be calculated from the inverse of the successful jump frequency, $t_{obs} = 1/\Gamma$; the latter has been developed by Zheng et al. [18] to be

$$\Gamma = \frac{\nu_0 b}{l_{obs}} \exp \left( -\frac{\Delta F}{kT} \right) \sinh \left( \frac{r \Delta V}{kT} \right)$$

(8)

where $\nu_0$ is the frequency of attempts of dislocations to jump the energy barrier, $l_{obs}$ the average obstacle spacing, $\Delta F$ the activation energy, $k$ the Boltzmann constant, $T$ the temperature (K) and $\Delta V$ the activation volume. It has been shown [18] that high activation energy or small activation volume leads to a large obstacle escape time. The thermal-activation enhanced DDP model together with the slip transfer methodology presented here are utilised in the next sections to examine the well-known size effect in polycrystals in order to present an assessment of the new approach. This is then followed by an investigation of GB slip transfer in cold dwell fatigue for which dislocation pile-up, thermally-activated dislocation escape, and potentially GB slip transfer in the hard-soft grain combination are controlling mechanisms.

4. Grain size strengthening (size effect) for impenetrable and penetrable GBs

The discrete dislocation plasticity model incorporating slip transfer is utilised first to assess the grain size strengthening size effect in a titanium alloy. Three selected average grain sizes, (0.25, 0.50, 1.00) $\mu$m, are chosen as in Li et al. [39] and assessed under uniaxial, displacement-controlled loading along the x-
direction depicted in Fig. 8. The model sample dimensions are 3μm × 9μm and 40 × 120 quadratic finite elements are employed to solve the boundary condition correction problem [46]. The crystal morphology is generated using a controlled Poisson Voronoi tessellation employed by VGRAIN software [47] (see Fig. 8). The modelling parameters and material properties were obtained by Zheng et al. [17] based on independent cyclic fatigue loading experimental data of Ti-6242 alloy. These parameters, as detailed in Table 1, enable the DDP model to reproduce the rate-sensitive responses under uniaxial tension and predict the load shedding during dwell fatigue loading conditions. In this size effect study, only a-prismatic slip systems are considered, i.e. the c-axis of the HCP unit is oriented perpendicular to the loading direction.

Two different strain rates are considered: at high strain rate, \( \dot{\varepsilon} = 10^3\,s^{-1} \), the dislocation behaviour is mainly controlled by nucleation and free flight, and at low strain rate, \( \dot{\varepsilon} = 10^{-4}\,s^{-1} \), the movement of the dislocations is predominated by the thermally activated escape from pinned obstacles. The stress-strain responses of impenetrable and penetrable GBs under these two strain rates are compared in Fig. 9. Generally, the Hall-Petch effect, i.e. increasing flow stress for smaller grains sizes, is observed in both the impenetrable and penetrable GB models under both strain rate regimes. The flow stress for the case of penetrable GBs is always lower than that for impenetrable GBs with the same morphology.

Under a high strain rate such as that used in Li et al. [39], the effect on the overall plastic response of slip penetration is found to be reduced to a negligible level when the grain size is increased to 1.00μm. In order to understand the differences for different types of grain boundaries, the slip contours of two selected grain sizes at high strain rate are compared in Fig. 10. The slip \( \xi \) is defined as the summation of the resolved shear strain \( \gamma \) on all slip systems, i.e. \( \xi = \sum_{\gamma = 0}^{\gamma \neq 0} \). For impenetrable GBs for small and large grain sizes, Fig. 10(a) and (b), strong slip bands are seen to form within individual grains, in different directions. However when dislocation transmission is permitted, Fig. 10(c) and (d), continuous slip bands are much more frequently developed across the entire polycrystal. It can be seen that the continuous slip bands are normally formed across adjacent grains with small misorientations, confirming that the dislocations penetrate the GBs more easily if the GB energy barrier is lower.

At low strain rate, in Fig. 9(b), the flow stress spacing resulting from impenetrable and penetrable GB models are found not to depend strongly on the grain size. Distributions of the stress component \( \sigma_{xx} \) with the dislocation structure shown at \( \varepsilon = 0.05 \) under low strain rate \( \dot{\varepsilon} = 10^{-4}\,s^{-1} \) are shown in Fig. 11. For the impenetrable GB polycrystal models with grain size \( d = 0.25\mu m \) and 1.00μm, stress is concentrated at the grain boundaries and the associated dislocation structures show strong pile-ups at these boundaries. The stress concentration is stronger in small grain sizes due to the high density of grain boundaries. In contrast, the stress distribution is more uniform in the penetrable GB polycrystal models for both grain sizes. The dislocation transmission across boundaries enables the development of continuous slip bands and the stress concentrations resulting from the pile-up groups are diminished. The dislocations transmit through grain boundaries and eventually leave the specimen from the free surfaces.

5. Slip transfer in cold dwell fatigue

In this section, we focus on the effect of slip penetration in terms of load shedding at hard-soft grain combinations in Ti-6242 oligocrystals which has been argued to be a key factor in controlling the dwell fatigue debit in several titanium alloys [6,10,16,17,49]. The rate-sensitive discrete dislocation formulations with and without slip transfer are utilised to address the dwell fatigue response, and a schematic diagram of the polycrystal model setup is shown in Fig. 12. The model sample dimensions are 10μm × 10μm, which is subjected to a uniaxial stress-controlled loading in the y-direction as indicated. The loading history is shown in Fig. 12(d), in which the maximum applied stress magnitude is chosen to be 0.95 of the macroscopic yield stress \( \sigma_{yy} \), i.e. \( \sigma_{yy} = 0.95\sigma_{yy} \), which is deemed most relevant for in-service conditions. The crystal morphology is created using the VGRAIN software [47] with an average grain size of 5μm², with minimum and maximum grain size 3μm² and 7μm² respectively, with regularity parameter 0.95. A soft-hard grain combination is located in the central region of the model for which the crystallographic orientations are shown in Fig. 12(c). The other surrounding grains are chosen to be relatively soft, i.e. their c-axes are chosen to be perpendicular to the loading direction. The grain boundaries between soft and hard grains use the ATGB energies shown in Fig. 4 and the soft-hard grain boundaries use the STGB energies shown in Fig. 3. Preliminary calculations are carried out with \( \omega = 1 \). In order to obtain detailed and accurate solutions of the stress and displacement fields, the finite element mesh was refined around the soft-hard grain combination, as shown in Fig. 12(b), with a minimum element size of 0.005 μm.

The polycrystal is subjected to uniaxial loading along the y direction and the yy-stress (equivalently the basal normal stress in the hard grain) distribution along the A – A’ path as shown in Fig. 12(c) is recorded during the loading history. The stress along the path is strongly affected by the position of A – A’, hence an average of the yy-stress along 20 paths parallel to A – A’ and within the shaded area shown in Fig. 12(c) is utilised to assess the stress throughout the soft-hard grain combination. The resulting average yy-stresses along path A – A’ before (in blue) and after (in red) the stress hold with and without GB slip transfer are shown in Fig. 13. The stresses, both within the grains and at the hard-soft grain boundary, are very similar at the beginning of the stress hold for both penetrable and impenetrable GB models. Then significant load shedding is observed in both cases at the end of the stress hold, but it is observed that the peak stress at the hard-soft grain boundary is considerably higher after the dwell period for the penetrable GB case for which slip transfer is permitted, compared to the impenetrable GB model. The stress is redistributed from the soft grain to the adjacent hard grain during the stress dwell, which leads to the

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**Table 1**

| General material parameters | \( G \) (MPa) | \( v \) | \( b \) (nm) | \( \rho_{dis} \) (μm\(^{-2}\)) | \( \sigma_{0.2} \) (MPa) |
|-----------------------------|-------------|------|-------------|----------------|------------------|
| 29022                       | 0.46        | 0.32 | 200         | 830            |                  |

| Mobility and nucleation     | \( B \) (Pa·s) | \( \eta \) (Pa·s) | \( \tau_{nuc} \) (MPa) | \( \rho_{nuc} \) (μm\(^{-2}\)) |
|-----------------------------|-----------|----------------|-------------------|------------------|
| \( 10^{-4} \)               | 908       | 480            | 10                |                  |

| Thermal activation          | \( \varepsilon_0 \) (K) | \( k \) (K\(^{-1}\)) | \( T \) (K) | \( \Delta \rho \) (J/atom) | \( \Delta V \) (Pa) |
|-----------------------------|-----------------|----------------|---------|-----------------|-------------|
| \( 10^{11} \)               | 1.38 × 10\(^{-23}\) | 293            | 9.8 × 10\(^{-20}\) | 0.5b\(^{3}\) |
significant increase of soft-hard grain boundary stress, which has been argued to be important in the facet nucleation process within the hard grain in cold dwell fatigue. When slip penetration is permitted in the polycrystal model (with $\omega = 1$), more plastic deformation is allowed to develop in the soft grains compared to the impenetrable model (exactly how this occurs is discussed in greater detail below). This is assisted by the slip transfer, but it does not significantly change the deformation in the hard grain because of its near-elastic behaviour. Since additional plasticity occurs in the soft grain, over and above that for the impenetrable polycrystal model, the load shedding in the slip penetration model is stronger.

The spatial distributions of $\gamma y$-stress and dislocation structure at the end of the stress dwell for impenetrable and penetrable GB models are shown in Fig. 14. Large numbers of dislocations are generated in the soft grain but only limited numbers of dislocations

![Fig. 9. Stress-strain responses of polycrystals of differing average grain sizes with impenetrable and penetrable GBs under the strain rates of (a) $10^3 \text{s}^{-1}$ and (b) $10^{-4} \text{s}^{-1}$.](image)

![Fig. 10. The distribution of total slip $\zeta$ for two selected grain sizes (a)/(c) $d = 0.25 \mu m$ and (b)/(d) $d = 1.00 \mu m$ at high strain rate $\dot{\varepsilon} = 10^3 \text{s}^{-1}$ with (a)/(b) impenetrable GB and (c)/(d) penetrable GB.](image)

![Fig. 11. The distribution of the stress component $\sigma_{xx}$ and the corresponding dislocation structures in (a)/(c) $d = 0.25 \mu m$ and (b)/(d) $d = 1.00 \mu m$ specimens at low strain rate $\dot{\varepsilon} = 10^{-4} \text{s}^{-1}$. The grain boundaries are impenetrable in (a)/(b) and penetrable in (c)/(d).](image)

![Fig. 12. (a) The DDP model geometry together with the crystal morphology; (b) the finite element mesh in the DDP model which is refined around the soft-hard grain combination; (c) local crystallographic orientations of the grain combination; (d) stress dwell loading history with $\sigma_{app} = 0.95\sigma_{0.2}$.](image)
can be seen in the hard grain. This leads to a much lower stress level in the soft grain (see Fig. 13). In the impenetrable GB model, as shown in Fig. 14(a), the dislocations in the hard grain are generated from the nucleation of Frank-Read sources in the hard grain itself, i.e. due to indirect slip transfer. The activated slip systems in the hard grain include \( c+a \)-pyramidal planes (indicated by black arrows) and \( a \)-basal planes (indicated by the blue arrow). These dislocations are nucleated from the sources located in high stress areas, which occur primarily near the grain boundaries. For the penetrable GB model, in addition to the indirect slip transfer, direct slip penetrations on the \( a \)-basal plane (indicated by the black hollow arrow) are also observed. Dislocations on that basal slip plane were originally nucleated from the sources on the \( a \)-prismatic slip plane in the adjacent soft grain. There is no direct slip transfer to the \( c+a \)-pyramidal slip systems because of the high energy barrier due to the difference in Burgers vector magnitude and the large misorientation angle.

The dislocations that arise due to slip transmission and re-emission are plotted in Fig. 15 together with the dislocation debris (i.e. only dislocations associated with GB slip transfer are shown). The first observation is that most of the slip penetration occurs at very particular grain orientation pairs, because these grains have low misorientation. In the case of penetration, a dislocation from a pile-up in the parent grain has overcome the grain boundary energy barrier and is transmitted in part to an adjacent grain, and may eventually escape at the nearest free surface. The back stress on the source that generated the transmitted dislocation is reduced by this process, hence the source is able to nucleate again which replaces the penetrating dislocation in the pile-up and the process is able to repeat; after enough dislocations transmit across a GB, the residual dislocation content accumulates to the point that re-emission is also possible. The GB penetration dislocation content, which is additional to the background dislocation content, enhances the load shedding and is clustered near the grain boundaries, hence leads to a higher peak stress at the soft-hard grain boundary at the end of the stress dwell.

In order to investigate the sensitivity of dwell response to the GB penetration energy given in equation (4), the dwell analysis study has been carried out over a range of values of \( u \). The magnitude of additional load shedding, i.e. the \( \sigma_{yy} \)-stress increases during the hold period at the soft-hard grain resulting from differing slip penetration energies, shown by selected values of \( u \) is plotted in Fig. 16. Higher values of \( u \) give energy barriers for slip penetration which are also higher, and \( u = \infty \) represents the case of an impenetrable GB. The peak stress increase resulting from dwell is found to be at least two times higher when dislocation transmission is permitted. Lower energy barriers allow more plastic deformation to occur within the adjacent soft grains during the stress hold and hence lead to stronger load shedding. The full mechanistic basis of dislocation activity at the grain boundaries in titanium alloys is complex, and more accurate representations of

![Fig. 13. The \( \sigma_{yy} \)-stress along the A–A’ path for the impenetrable and penetrable GB models before and after the dwell.](image)

![Fig. 14. The \( \sigma_{yy} \)-stress contours and corresponding dislocation structures in the soft-hard grain combination after the dwell for (a) impenetrable and (b) penetrable GB models (\( u = 1 \)). Indirect slip transfer in the hard grain is indicated by black solid arrows for \( c+a \)-pyramidal slip and the blue solid arrow for \( a \)-basal slip. Direct slip transfer on the \( a \)-basal slip plane in the hard grain is indicated by the black hollow arrow. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image)

![Fig. 15. Only the dislocations associated with GB penetration (transmitted and re-emitted dislocations, and the dislocation debris) are shown. The slip systems in each grain are also shown.](image)
the GB penetration energy barrier may be obtained in future analysis, but the significant effect of slip transfer on the dwell fatigue problem is well demonstrated here. It is interesting to note from Fig. 16 that significant increases in GB penetration energy (from one to four times the GB static energy) give little change to the load shedding until it becomes very large indeed effectively inhibiting slip transfer altogether.

During the forging processing of titanium alloys, a set of neighbouring individual grains with similar/common crystallographic orientation may be produced, which are known as macrozones or micro-textured regions (MTRs) [50]. The macrozone is similar to a very large effective region of uniform crystallographic orientation, and it has been argued that the existence of macrozones is important to dwell fatigue [1,51]. Lunt et al. [52] characterised the macrozone region in alloy Ti-6Al-4V using electron backscatter diffraction (EBSD) techniques and found in that region the c-axis in the macrozone to be parallel to the transverse direction (TD) as shown in Fig. 17(b). When the alloy is subjected to loading along TD, the macrozone behaves like a large effective hard grain. A polycrystalline model as shown in Fig. 17(a) with impenetrable and penetrable GBs is established in order to investigate the role of slip transfer under dwell fatigue loading with the existence of macrozones. For reasons of computational efficiency, the model dimensions are taken to be 200µm × 200µm with an average grain size of 8µm. The width of the macrozone is about 15µm. The same dwell fatigue loading as shown in Fig. 12(d) is applied on the top surface while the left and bottom surfaces are constrained as shown in Fig. 17(a). Two regions of interest are selected as shown in Fig. 18(a) and the yy-stresses after stress hold are shown in Fig. 18(b–d) for the cases of impenetrable and penetrable grain boundaries. In region 1, the stresses at soft-soft grain boundaries are overestimated due to the pile-ups at these boundaries when dislocation transmission is prohibited. On the contrary, the local basal-normal stresses at soft-hard grain boundaries in region 2 are amplified when dislocation transfer is permitted during dwell. Significant load shedding is found to occur to the hard-orientated macrozone, but no significant size effect is found to occur with respect to the previous analyses for polycrystal response in the absence of a macrozone. However, high peak basal stresses are developed within the macrozone as before potentially facilitating quasi-cleavage facet formation. In the case of the macrozone, a nucleated facet which is considerably larger than that for a non-macrozoned grain ensemble becomes possible and it may be that it is simply the larger initiation size which is most detrimental to component structural integrity arising in the presence of macrozones.

6. Conclusions

Atomistic simulations were used to determine the static grain boundary energies of STGB and ATGB in titanium as a function of misorientation angle and grain boundary orientation. The grain boundary energies were then utilised in a discrete dislocation model which explicitly includes thermally activated escape of pinned dislocations and incorporates slip transfer across grain

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1 The highest ratio between dislocation transmission barrier and static grain boundary energy reported in Ref. [37] is about 3. Since the energy barrier for dislocation transmission in Ref. [37] is normalised by volume, it is multiplied by one Burgers vector magnitude for direct comparison with the static grain boundary energy.
boundaries. The DDP model was first used to predict the grain size strengthening size effect in a titanium alloy at high strain rate (mobility and nucleation predominated) and low strain rate (thermal activation process controlled). A classic grain size strengthening effect was observed at both high and low strain rates. The results for polycrystals for which grain boundary slip transfer is permitted according to energy and geometric criteria were compared to corresponding impenetrable models. It was shown that the flow stress is lower when slip penetration is allowed; the effect of GB penetration is more significant in small grain size polycrystals.

The DDP model was then used to investigate the load shedding phenomenon in Ti-6242 alloy under dwell fatigue loading. It was shown that significant stress redistribution occurs within soft-hard grain pairs during the stress dwell period leading to significantly elevated grain boundary stresses at the end of the dwell, and very localised high basal stresses in the hard grain. The peak stress at the soft-hard grain boundaries for which slip transfer is permitted was observed to be significantly higher than in corresponding impenetrable grain boundary cases, i.e. the results indicate that the incorporation of slip transfer at soft-hard grain boundaries amplifies the stress redistribution by enhancing plastic slip in the soft grains, hence the load shedding effect, in cold dwell fatigue in susceptible Ti alloys. It was also observed that the slip penetration occurred across grain pairs with low misorientation, which are located close to a free surface. However, the key controlling mechanism with respect to load shedding in titanium alloys remains the time constant associated with the process of thermally activated dislocation escape; dislocation-grain boundary penetration is important and exacerbates the dwell load shedding, but plays a secondary role. The magnification of static GB energy to represent the transmission energy barrier has been demonstrated to have a small effect on load shedding in titanium alloys, Int. J. Fatigue 30 (2008) 2127–2139. Z. Zhang, M.A. Cuddihy, F.P.E. Dunne, On rate-dependent polycrystal deformation: the temperature sensitivity of cold dwell fatigue, Proc. R. Soc. Lond. Math. Phys. Eng. Sci. 471 (2015).

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