Slip band and grain boundary interactions in commercial purity titanium

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Abstract

The interaction between slip bands and grain boundaries in commercial purity titanium was examined using cross correlation based electron back scatter diffraction. At low strain level, three types of interactions were observed: blocked slip band with stress concentration; slip transfer; blocked slip band with no stress concentration. Stress concentration induced by the blocked slip band was fitted with Eshelby's theoretical model from which a Hall Petch coefficient was deduced. It was found that the Hall Petch coefficient varies with individual grain boundary. We investigated the geometric alignment between the slip band and various slip systems to the neighbouring grain. Stress concentration can be induced by the blocked slip band if the slip system is poorly aligned with $\langle a \rangle$ prismatic, pyramidal or basal slip systems in the neighbouring grain. Transfer of slip across the boundary occurs when there is good alignment on $\langle a \rangle$ prismatic or $\langle a \rangle$ pyramidal slip systems. Other stress relieving mechanisms are possible when the best alignment is not with the slip system that has lower critical resolved shear stress (CRSS).

Keywords:

HR-EBSD; Slip transfer; Slip band; Hall-Petch coefficient; Titanium

1. Introduction

Grain boundaries are effective barriers to dislocation motion providing a substantial strengthening mechanism for polycrystalline materials [1]. The pile-up of dislocations against grain boundaries could lead to localised high intensity stress concentrations, especially in planar slip materials. The forward stress generated by slip band/grain boundary interaction is cited to lead to slip transfer [2], deformation twin nucleation [3, 4], cavity nucleation [5], fatigue crack nucleation [6], and some other phenomena [7, 8].

The back stress of a pile-up, which results from cumulative stress fields from each individual dislocation and therefore depends on the size of the pile-up and the number of dislocations in it, tends to counteract the externally applied stress. This leads to a lower resultant stress state for dislocation slip [9]. Such a model has been widely used as an explanation for the empirical Hall-Petch relationship [9-11] which relates yield strength to grain size of a polycrystalline material by the equation: $\sigma_y = \sigma_0 + kD^{-\frac{1}{2}}$, where D is the average grain diameter. The 'friction stress' σ_0 is the stress required to sustain dislocation motion in the interior of a grain [12, 13], while the $kD^{-\frac{1}{2}}$ term is the grain boundary contribution to yield strength [12]. k is often referred to as the Hall-Petch coefficient, and usually captures the average effect of the grain boundaries in the polycrystal. A recent reassessment of much of the literature data concerning grain size effects on yield strength by Dunstan and Bushby [14] has cast doubt on the Hall-Petch relationship, and attempts to rationalize it with other size effects.

The Hall-Petch coefficient has traditionally been obtained by mechanical testing of samples with varying grain diameter. Hyun et al [15] have reported $k = 0.25 \text{ MPam}^{0.5}$ for grade 2 commercially pure titanium (CP-Ti) deformed at room temperature under tension. While Lederich et al [16] found $k = 0.18 \text{ MPam}^{0.5}$ and $k = 0.40 \text{ MPam}^{0.5}$ for pure Ti deformed under

tension at 575K and 295K respectively. For room temperature compression Salem et al [17] reported $k = 0.67 \text{ MPam}^{0.5}$ for CP-Ti. Although $\sigma_y = \sigma_0 + kD_{GB}^{-1/2}$ has now been shown to support macro-mechanical testing data better than the Hall-Petch equation [14], the Hall-Petch coefficients available in the literature do allow the overall effects of crystal structure, alloying additions and other factors on the relative effectiveness of grain boundary strengthening to be assessed. Of course it is to be expected that the nature and geometry of individual grain boundary types should have a pronounced effect on the intensity of local stress concentrations generated [18, 19]. Amongst others, Sangid et al [20] suggest that the slip band and grain boundary interaction is strongly affected by the character and structure of grain boundaries. This leads to the thinking that boundaries of different characteristic should have different resistance to slip transfer. Therefore, an investigation into the strengthening mechanisms of individual grain boundaries is of theoretical and practical importance.

A large body of theoretical and modelling work has been focused on predicting the resistance to slip transfer using boundary related parameters as has been reviewed by Morris [21]. Some of the proposed models require grain boundary parameters that cannot be directly measured, while others contain parameters that depend on pre-knowledge of k , rendering those models descriptive but not predictive. The research of Beta et al [13] suggested a relatively independent model but this suffers from difficulties of accurately determining grain boundary strain energy and ignores stress concentrations that might arise near grain boundary. Theoretical work by Eshelby, Frank, and Nabarro [22], on the equilibrium spacing of dislocations, proposed a solution to modelling the stress concentration as a result of slip band-grain boundary interactions. This model, illustrated in figure 1, consists of an array of edge dislocations blocked by a grain boundary. This causes a stress concentration at the tip of the slip band in the neighbouring grain. This stress concentration, when resolved to the shear plane of the pile-up, attenuates in a 'one over square root distance' fashion directly ahead of the pile-up away from the grain boundary. The resolved shear stress τ can thus be written as

$$\tau = \tau_0 + \frac{K}{\sqrt{r}} \quad (1)$$

where K describes the stress intensity of the stress field and r is the distance from the grain boundary.

Figure 1: Eshelby's model of dislocation pile-up at grain boundary. The red curve to the right of grain boundary represents stress distribution ahead of the blocked slip band.

Britton et al [23] recently mapped the stress distribution near the head of a blocked slip band using the High Resolution EBSD (HR-EBSD) technique [24, 25] and found the stresses to be consistent with the Eshelby-Frank-Nabarro model. The stress intensity factor K can be obtained by curve fitting of the resolved shear stress line profile ahead of the pile-up. This study provided a method to directly measure the stress intensity factor associated with an individual selected slip band-grain boundary interaction. It is therefore important to extend such measurement to different slip band/grain boundary interactions for a systematic evaluation of the strength of grain boundary in terms of the alignment between crystal slip systems.

The stress concentration accumulated by the dislocation pile-up can be redistributed along grain boundary if the Burger's vector of grain boundary dislocation dissociated from matrix dislocation is within the boundary plane in which it can then glide. This grain boundary gliding mechanism was described in [26, 27]. If the grain boundary dislocations have a component out of its boundary plane then ledges can be created which can in turn lead to the nucleation

of boundary cracks [28]. This has been observed by Lee et al [29] via an in-situ TEM study. The most common stress relief mechanism is by generating new dislocations in the neighbouring grain [30-36].

This could be done by several experimentally observed mechanisms:

(1) direct transfer, when the incoming slip plane share a common intersection with the outgoing slip plane on grain boundary, and the Burger's vectors of both slip systems are equal, i. e. this transfer mechanism leaves no residual Burger's vector at grain boundary.

(2) transfer with residual grain boundary dislocation. This mechanism is accomplished by dislocation absorption and subsequent re-emission. The emitted dislocations could either connect to the previous slip band or be displaced along grain boundary [34]. An energy barrier proportional to the magnitude of residual Burger's vector was proposed to play a crucial role in this type of transfer mechanism [20, 36];

(3) New dislocation sources could be activated due to local stress concentration generated around the tip of a blocked slip band. For this type of dislocations to glide across the whole grain, resolved shear stress on their slip plane should be sufficiently large otherwise they cease propagating after a short distance from grain boundary and other more mechanically favourable dislocation sources could be activated [10, 11, 36].

Early research by Livingston and Chalmers [33] attempted to predict which slip system is more favourable during a slip transfer process, and for this purpose a criteria was proposed:

$$N_{ij} = [(e_i \cdot e_j)(g_i \cdot g_j) + (e_i \cdot g_j)(e_j \cdot g_i)] \quad (2)$$

Where $\mathbf{e}$ is slip plane normal and $\mathbf{g}$ is slip direction. The subscriptions i and j represent two slip systems on either side of a grain boundary. Slip transfer is likely to take place on the system having a high N_{ij} value. This criterion emphasise the importance of geometric alignment on the choice of transferred slip system. Later work by Shen et al [31] pointed out the importance of incorporating a resolved shear stress on slip transfer and a new model was proposed:

$$N'_{ij} = (\mathbf{L}_i \cdot \mathbf{L}_j)(\mathbf{g}_i \cdot \mathbf{g}_j) \quad (3)$$

Where $\mathbf{L}$ is the lines of intersection between grain boundary plane and the planes of incoming (subscript i) and outgoing (subscript j) slip systems. A schematic showing the geometry of the slip plane alignment can be seen in figure 2.

Figure 2. A schematic showing geometric configurations between two slip systems intersecting a grain boundary. $\mathbf{L}$ is the line of intersection between slip plane and grain boundary, $\mathbf{n}$ is plane normal, and the burgers vector $\mathbf{b}$ is used to represent the slip direction $\mathbf{g}$.

Slip transfer is again favoured for slip systems with highest N'_{ij} , i.e. the angles between $\mathbf{L}_i$, $\mathbf{L}_j$ and $\mathbf{g}_j$, $\mathbf{g}_i$ should be minimized. The transferred slip plane therefore is the one that maximize

N'_{ij} and the slip direction is the one that have highest resolved shear stress. While this model was successful in predicting all four boundary/pile-up configurations studied by Shen, exceptions were found by Lee et al [35] that, in some cases, systems that generate large grain boundary dislocations cease to operate even when the resolved shear stress is highest. Taking into account this issue, the slip transfer criteria suggested by Lee, Robertson, and Birnbaum (LRB criteria) consists of three aspects:

- (1) the geometric alignment factor N'_{ij} as shown in equation 3 should be maximized;
- (2) the magnitude of residual Burgers vector as the difference between incoming and outgoing dislocations should be minimized;
- (3) the resolved shear stress on the outgoing slip system imposed by the incoming slip system should be maximized.

Although derived from a study of FCC metals, the LRB criteria has had some success in studying slip transfer process in hcp titanium alloys [37].

The first and second points in LRB can be combined if Burgers vector, $\mathbf{b}$, is used to describe the slip direction, $\mathbf{g}$, in equation 3. In reality, equation 3 is difficult to apply because in current experimental condition it is not easy to determine $\mathbf{L}$.

As an alternative, Werner et al [38] suggested that slip plane normal $\mathbf{n}$ could be used to replace $\mathbf{L}$ as the angle between slip plane normal could never exceeds the angle between intersection lines with grain boundary irrespective of the grain boundary orientation. Therefore an alternative equation taking account of both geometric alignment and residual Burgers vector can be written as:

$$M = \frac{(\mathbf{n}_i \cdot \mathbf{n}_j)(\mathbf{b}_i \cdot \mathbf{b}_j)}{|\mathbf{b}_i||\mathbf{b}_j|} \quad (4)$$

Where $\mathbf{n}$ and $\mathbf{b}$ are slip plane normal and Burgers vector respectively.

In this research, the factor M in equation 4 will be employed to investigate local slip system alignments and the correlation between M and the stress intensity factor for a collection of slip band/grain boundary pairs will be analyzed. Furthermore, a comparison of the M factors will be made between grain boundaries with and without the occurrences of obvious slip transfer. The results are interpreted together with resolved shear stress on various slip systems.

2. Materials and experimental procedures:

The material used in this research was commercial purity titanium supplied by Timet UK Ltd. The chemical composition is listed in table 1 [23]. Tensile test pieces with a gauge dimension of 30mm x 3mm x 1mm were cut using electron discharge machining. The long axis of the tensile piece was along the rolling direction of the as received bar. The tensile pieces were heat treated in vacuum at 830°C for 24 hours to grow the grain size to an average of ~300 μm . Samples were then ground using silicon carbide paper down to 4000 grit followed by chemical-mechanical polishing using 50nm colloidal silica suspension. The colloidal silica polishing was followed by etching using a solution with 1% HF and 10% HNO_3 in water to remove the oxide and hydride layers which severely degrade the quality of electron back scattered patterns. This polish-etch-polish process was repeated until a crisp grain boundary structure was visible in optical microscope with polarized illumination.

Element	Fe	O ₂	N ₂	C	Ti
Composition	0.35 wt%	700ppm	35ppm	0.01 wt%	Balance

Table 1. Chemical composition of the as received grade 1 commercially pure titanium[23].

The sample was deformed in tension to 1% plastic strain measured by in-situ digital image correlation. The applied stress reached a maximum value of 235 MPa. EBSD maps featuring various slip band/grain boundary interactions were acquired including a number of boundaries with blocked slip bands and a number of boundaries with transferred slip bands using JOEL JSM 6500 scanning electron microscopy. The maps had an average size of 10 μm x 25 μm and were obtained at 20 KV with 14 nA beam current over a square array of 0.2 μm step size. At each interrogation point the back-scattered electron diffraction pattern, consisting of 1000

x 1000 pixels, was captured and saved as TIFF image format with 12-bit depth using OIM Data Collection V5.

For cross correlation, the patterns were transformed into the Fourier domain and filtered to remove high frequency noise and low frequency background gradients. For each grain a reference point was picked towards the interior of the grain, where it was assumed that the stress state was relatively low and uniform. For each pattern, 50 regions of interest with 256 x 256 pixel size were selected with one at the middle of the pattern, 19 others surrounding it in a ring and the remaining 30 randomly distributed. These region of interests on test patterns were compared with the corresponding parts on the reference pattern using cross-correlation [39] with which pattern shifts as small as 0.02 pixels can be detected [40]. These pattern shifts were used to fully determine the displacement gradient tensor (DGT) using the assumption that the stress perpendicular to the sample surface is zero [41]. Locally the lattice rotations could be quite large and so the pattern remapping algorithm developed by Britton and Wilkinson [25] was used. This involves using a first pass of cross-correlation analysis to estimate a finite lattice rotation which is used to remap the test pattern intensities in a virtual reorientation of the test region. A second pass of cross correlation analysis is then used to determine the lattice strains and a correction to the lattice rotation. The DGT from the first and second passes are combined to give a total deformation gradient $\mathbf{F}$ from which the Green strain tensor ($\mathbf{E}$) was obtained: $\mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{I})$. These elastic strain fields were then used to calculate stress fields using elastic constants (in GPa) for titanium: $C_{11} = 162.4$ $C_{33} = 180.7$ $C_{44} = 117$ $C_{66} = 35.2$ $C_{13} = 69.0$ [42]. Polar decomposition of $\mathbf{F}$ into the product of rotation and stretch tensors using singular value decomposition methods enables the lattice rotation to be determined. These finite rotation tensor were used to estimate 6 infinitesimal rotation gradients using procedures documented in [23] and linked to 6 out of 9 components of Nye's dislocation tensor [43]. The remaining 3 components are associated with lattice rotation gradients along the depth of the sample and therefore can only be determined using 3D

profiling technique. The GND density presented in this paper is therefore a lower-bound estimation.

For GND calculation of α -Ti the following dislocation types were used: 3 $\langle a \rangle$ screw and 6 $\langle c+a \rangle$ screw; 3 $\langle a \rangle$ edge on basal plane; 3 $\langle a \rangle$ edge on first order prismatic plane; 6 $\langle a \rangle$ edge on first order pyramidal plane; 12 $\langle c+a \rangle$ edge on first order pyramidal plane [44]. The GND density for each type of dislocation is found using a standard linear programming algorithm by minimizing the possible total GND line energy [45].

It is important to note that the absolute strain state of the reference pattern is unknown. Therefore the elastic strains presented here are relative values. However, this uncertainty does not affect the GND density as it is only related with lattice curvatures [46].

The EBSD code initially reports stresses in the external sample reference frame. For slip band/grain boundary interactions that lead to stress concentration these stresses were rotated such that the shear stress on the slip plane of the deforming grain in the Burgers vector direction was obtained across the two grains. From the rotated resolved shear stress field, line profiles were extracted along the direction of the pile-up. The stress intensity factor K was then determined by fitting the stress line profile using non-linear method to the equation proposed in [23]:

$$\sigma_{31}^r = A + K/\sqrt{X + B} \quad (5)$$

Where σ_{31}^r is the resolved shear stress imposed by the dislocation pile-up in the neighbouring grain, X is the distance along the line profile away from grain boundary. The constant A is introduced to allow for uncertainty of stress state at the reference point while the constant B is introduced to allow for the uncertainty of grain boundary position.

For a number of the blocked slip bands atomic force microscopy (AFM) was used to determine the height of the slip bands. A Pacific Nanotechnology Nano-R with SPM Cockpit model AFM was used in contact mode to map the surface topography over regions 45 μ m by 45 μ m. Images

were analyzed on-line and topography changes across the slip band averaged over several points along the slip band.

3. Results

Analysing the HR EBSD data from many slip band-grain boundary intersections allow us to identify three broad categories of slip band-grain boundary interactions. These were:

(1) blocked slip band with a stress concentration ahead of it; (2) slip transfer where the slip band in one grain leads 'directly' to a slip band in the neighbouring grain; (3) a blocked slip band with no long range slip band in the neighbouring grain but no obvious stress concentration. We give results for each category in the next three sections.

3.1. Blocked slip band that lead to stress concentration:

This type of interaction features a blocked slip band in one grain with no macroscopic slip transfer into the neighboring grain, observed from surface topography, but localized stress concentration around the intersection point between slip band and grain boundary observed with HR-EBSD.

One example of such interactions is shown in figure 2. The slip band was formed to accommodate macroscopic tensile loading (for all images in this paper the tensile direction is horizontal with respect to the image) as is revealed on the EBSD image quality map (figure 2a). No slip transfer or slip band formation was observed in the neighboring grain. The orientation relationship between the two grains is close to a 70° rotation about x_1 axis as is revealed by the superimposed unit cell structures. The slip plane of the slip band was found by trace analysis and the crystal orientation from EBSD and is indicated in red color. This slip system corresponds to a low CRSS $\langle a \rangle$ prismatic slip system that has a high (0.50) Schmid factor. HR EBSD output of the full elastic stress tensor is illustrated in figure 2 b. Stress concentration induced by the blocked slip band is revealed most clearly in the σ_{11} and σ_{12} components. The stress tensor shown in figure 2 b is measured in sample frame as defined

by x_1 and x_2 (x_3 component is perpendicular to the image surface and pointing into the page).

Figure 2c shows a more useful axis system, x_1^r x_2^r x_3^r , which is described by the Burgers vector (x_1^r) and the direction perpendicular to it (x_2^r) of the active slip system. The resolved shear stress on the projection of the active slip plane is the σ_{13}^r component of the tensor, and is shown in figure 2 d.

(Figure 2 goes here)

Figure 2: (a) EBSD image quality map of a blocked slip band with grain orientation overlapped; (b) HR EBSD stress output; (c) Coordinate system defined on sample reference frame (x_1 x_2) and slip plane reference frame (x_1^r x_2^r x_3^r); (d) The σ_{13}^r component of the stress tensor after rotation, dashed line represent direction along which stress profile is extracted (all colour scales in GPa).

A line scan along the direction of the slip band on the upper grain but extended into the lower grain (indicated by the dashed line) was extracted and the resulting stress profile is shown in figure 3. These data points fit well with the model proposed by Eshelby et al [22].

Figure 3: Stress concentration ahead of the blocked slip band as in figure 2 d with comparison to the model described by Eshelby et al [22].

Fitting the experimental stress profile with equation 5 allows a K value of 0.78 (± 0.08) MPa $m^{1/2}$ to be obtained for this boundary, where the error indicates standard error from best fit parameters. The same procedure was performed for four other boundaries in this category.

Figure 4: Stress profile in front of blocked slip bands and fitted stress profiles. Solid line represents the position of incoming slip band and dashed line is the direction along which stress profile was extracted

The results are summarized in figure 4 which shows the resolved shear stress maps overlaid with corresponding grain orientations indicating different grain boundary geometries, along with the stress variation on a line directly ahead of the slip line. The K value, as obtained from fitting each stress profile with equation 4, is indicated for each grain boundary. The LRB criteria was employed in such a way that the combination of M factor (equation 3), between the incoming slip system and various of possible slip systems in the neighbouring grain, and the resolved shear stress (RSS), described by Schmid factor (S), were used to characterize each case of interaction. For all five slip band—grain boundary interactions in figures 2 & 4, trace analysis revealed that each of the slip bands were due to <a> prismatic slip. The best alignment (i.e. highest M) between these prismatic slip systems with possible <a> basal, <a> prismatic, <a> pyramidal, and <c+a> pyramidal slip systems and related Schmidt factors (S) are compiled in table 2.

	Boundary 1	Boundary 2	Boundary 3	Boundary 4	Boundary 5
	K=0.78	K=0.62	K=0.32	K=0.21	K=0.1
Prismatic→Prismatic	M ₁ =0.33	M ₁ =0.40	M ₁ =0.47	M ₁ =0.53	M ₁ =0.54
	S ₁ =0.23	S ₁ =0.49	S ₁ =0.40	S ₁ =0.30	S ₁ =0.28
	M ₂ =0.11	M ₂ =0.40	M ₂ =0.06	M ₂ =0.01	M ₂ =0.01

	$S_2=0.47$	$S_2=0.49$	$S_2=0.46$	$S_2=0.49$	$S_2=0.50$
Prismatic→Basal	M=0.35 S=0.23	M=0.48 S=0.01	M=0.23 S=0.03	M=0.28 S=0.14	M=0.33 S=0.01
Prismatic→ $\langle\alpha\rangle$ Pyramidal	M=0.48 S=0.02	M=0.6 S=0.33	M=0.49 S=0.25	M=0.56 S=0.17	M=0.61 S=0.20
Prismatic→ $\langle c+a \rangle$ Pyramidal	M=0.60 S=0.33	M=0.54 S=0.40	M=0.83 S=0.27	M=0.82 S=0.27	M=0.78 S=0.11

Table 2: Geometric alignment (M) between incoming slip plane and possible slip planes in neighbouring grain and Schmidt factor on corresponding slip system (S). Only the best alignments (i.e. highest M) are listed except for M_2 values in second row of prismatic→prismatic alignment.

For this category of slip band-grain boundary interactions, the incoming prismatic slip systems are better aligned (i.e. higher M) with $\langle c+a \rangle$ pyramidal slip system in adjacent grains, however the magnitude of the $\langle c+a \rangle$ Burgers vector is too large compared to $\langle a \rangle$ slip and transfer would require accommodation of additional $\langle c \rangle$. This coupled with the higher CRSS and generally low Schmid factor means slip is not transferred to $\langle c+a \rangle$ slip system. On the other hand, easy slip systems (prismatic) have poor alignment (i.e. low M) with low Schmid factor. Those easy slip systems that do have high Schmid factor, almost at the maximum value of 0.5, were however found to have the worst alignments with incoming prismatic slip systems.

The stress ahead of the blocked pile-up is likely to depend on the number of dislocations within the pile-up. The analysis of Eshelby et al [22] indicates that the stress intensity increases as $\sqrt{N}$ when the number of dislocations in the pile-up (N) is large. AFM maps, combined with the orientation of the active slip system, were used to measure the slip band heights h , from which N was obtained from knowledge of the Burgers vector length and slip direction established from EBSD. Figure 5 shows a plot of the measured stress intensity ahead of the blocked slip band as a function of $\sqrt{N}$ (equation 6). Boundary 3 (table 2) is not shown in figure 5 as the position of which on sample surface was lost. Instead, the result obtained by Britton et al [23] was incorporated in as is indicated by the triangular mark in figure 5.

Figure 5: K (stress intensity factor, MPa $\text{m}^{1/2}$) as a function of the square root of the number of dislocations, N , in the slip band. X axis corresponds to K' measured from AFM and Y axis K measured from HR-EBSD. Triangular mark is the data from previous research[23].

3.2. Slip band/grain boundary interactions that lead to slip transfer:

For this type of interaction, the slip band is transferred across the grain boundary (it is not clear whether it is direct transfer or not under the resolution of current experimental procedure). As ex-situ experiment does not tell which slip band is the incoming band and which is the outgoing band, it is necessary to resolve the stress tensor onto the slip plane for each individual slip bands. For one of the slip band/grain boundary interactions of this category, the σ_{13} variation is shown in figure 6.

Figure 6: Scanning electron microscopy image showing a slip transfer feature (left), and σ_{13} shear stress resolved onto the active slip system of the top grain (middle) and bottom grain (right).

It can be seen from the stress map that there are low level of diffuse stress variations near each slip band but no strong localized stress concentration like those in figure 2 was induced

by either of the slip bands. No ‘one over square root distance’ stress distribution can be observed ahead of either slip band. Seven instances where slip bands continued on either side of the grain boundary were mapped using HR-EBSD and in all cases there were no significant stress concentrations at the grain boundary. For geometric alignment investigation, slip band on prismatic plane was assumed to be the incoming slip band and the M factor and Schmidt factor S were calculated for the possible outgoing slip band, these are compared in table 3 for the possible slip systems in the ‘transferred’ grain.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
Prismatic→Prismatic	M ₁ =0.94 S ₁ =0.26	M ₁ =0.46 S ₁ =0.33	M ₁ =0.95 S ₁ =0.33	M ₁ =0.41 S ₁ =0.39	M ₁ =0.84 S ₁ =0.47	M ₁ =0.73 S ₁ =0.43	M ₁ =0.91 S ₁ =0.47
Prismatic→Basal	M=0.04 S=0.03	M=0.71 S=0.41	M=0.19 S=0.03	M=0.64 S=0.20	M=0.45 S=0.18	M=0.68 S=0.11	M=0.15 S=0.05
Prismatic→<α>Pyramidal	M=0.67 S=0.18	M=0.80 S=0.31	M=0.78 S=0.25	M=0.72 S=0.42	M=0.9 S=0.18	M=0.43 S=0.01	M=0.50 S=0.35
Prismatic→<c+a>Pyramidal	M=0.56 S=0.10	M=0.32 S=0.13	M=0.52 S=0.11	M=0.44 S=0.11	M=0.66 S=0.38	M=0.40 S=0.17	M=0.76 S=0.31

Table 3: Best alignment (maximum M) between prismatic slip system in one grain and various slip systems in the other grain. Coloured cells indicate the observed slip plane of the ‘transferred’ slip system.

By comparing the alignments in each column for the seven slip transfer cases, it can be seen that the observed ‘transferred’ slip systems are the ones that have the best geometric alignment (i.e. highest M) with the ‘incoming’ slip system. Transferred slip bands were formed on either prismatic slip plane or <α>pyramidal slip plane. The transferred slip systems also tend to have a relatively high Schmid factor based on the far field applied loading. This can be noticed by comparing the S values for each column of table 3.

3.3. Blocked slip band that does not lead to stress concentration:

The third category of slip band/grain boundary interaction appear similar to the first category (section 3.1) in that SEM imaging shows a slip band terminating at a grain boundary. The difference is that HR-EBSD reveals that these blocked slip bands do not lead to stress concentration. Two examples of the six cases mapped are shown in Figure 7.

Figure 7: Image quality map visualizing a blocked slip band, corresponding geometrically necessary dislocation (GND) density map (colour bar is on Log_{10} scale), and σ_{13}^r shear stress (GPa). Black dash line indicates slip trace.

The distinguishing feature for this category of interaction is that no localized stress concentration can be seen around the intersection of the slip band and the grain boundary as is revealed by the σ_{13}^r resolved shear stress fields in figure 7. We have also looked at the lower bound estimate of the GND density distributions for these cases. In one case (figure 7 (a)) there is localized GND concentration near the head of the blocked slip band which suggests an interaction in which some dislocation content is reflected back from the grain boundary. While in another case (figure 7 (b)) there is no localized GND concentration but some evidence of increased GND density distributed along grain boundary. The geometric alignments for the six instances of this type of interaction that were analysed are listed in table 4.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
Prismatic→Prismatic	$M_1=0.72$	$M_1=0.39$	$M_1=0.67$	$M_1=0.87$	$M_1=0.70$	$M_1=0.48$
	$S_1=0.35$	$S_1=0.34$	$S_1=0.44$	$S_1=0.27$	$S_1=0.48$	$S_1=0.38$
	$M_2=0.05$	$M_2=0.05$	$M_2=0.00$	$M_2=0.11$	$M_1=0.70$	$M_1=0.04$
Prismatic→Basal	$S_2=0.48$	$S_2=0.48$	$S_2=0.42$	$S_2=0.49$	$S_1=0.48$	$S_1=0.41$
	$M=0.58$	$M=0.70$	$M=0.39$	$M=0.39$	$M=0.49$	$M=0.53$
Prismatic→<a>Pyramidal	$S=0.04$	$S=0.09$	$S=0.07$	$S=0.04$	$S=0.13$	$S=0.28$
	$M=0.92$	$M=0.78$	$M=0.74$	$M=0.88$	$M=0.84$	$M=0.65$
Prismatic→<c+a>Pyramidal	$S=0.26$	$S=0.30$	$S=0.35$	$S=0.21$	$S=0.42$	$S=0.22$
	$M=0.50$	$M=0.41$	$M=0.64$	$M=0.60$	$M=0.68$	$M=0.58$
	$S=0.11$	$S=0.01$	$S=0.20$	$S=0.03$	$S=0.14$	$S=0.01$

Table 4: Best alignments (except for M_2 in prismatic→prismatic alignment) between the blocked slip plane and various slip systems in the neighbouring grain. Boundary 1 and Boundary 2 correspond to figure 7 (a) and (b) respectively.

From the comparison between the alignments with various slip systems, the blocked pile-up planes are better aligned with $\langle a \rangle$ pyramidal plane that have relatively lower Schmid factor. Prismatic slip systems, on the other hand, have generally both lower M value and Schmid factor, compared to the $\langle a \rangle$ pyramidal system. However the M and S values of prismatic slip systems are not so distinct from those grains in table 3 for cases where slip transfer did occur. Similar to blocked slip bands in the first category of interactions (table 2), prismatic slip system with higher Schmid factor have the worst alignment (M_2) with incoming slip bands.

3.4. Residual Burgers vector, stress intensity factor, and M

We have examined the data for correlation between category of interaction and residual Burgers vector between the incoming (prismatic) slip system and various slip systems in the neighbouring grain, stress intensity factor K, and geometric alignment factor M. For each of the three types of slip band - grain boundary interactions figure 8 plots the alignment factor M assuming transfer to either prismatic, or $\langle a \rangle$ pyramidal slip systems against the corresponding Schmidt factor S. The filled symbols on figure 8 represent the best aligned $\langle a \rangle$ prism slip system, while the hollow symbols are for the best aligned $\langle a \rangle$ pyramidal slip systems. The background red colouring (zone 3) of the plot indicates the general tendency for the cases where slip transfer was observed to combine both good alignment (i.e. high $M > 0.7$) and large shear stress (i.e. high $S > 0.3$) on the selected slip system. While blocked slip bands, leading to a measureable stress intensity, (blue background shading, zone 1) tended to be observed when the slip system alignment was relatively poor (M factor below ~ 0.5) but over the whole range of possible Schmidt factors. Blocked slip bands with very low induced stress intensity factors tend to be in a regime with intermediate M but most often with significant Schmidt factor. There is significant overlap between the three regions in this M-S space possibly due to the varying amount of slip on the different slip bands observed. It seems that although both M and S influence the situation the alignment factor M takes priority in controlling slip transfer.

Figure 8: The plot of Schmid factor (S) against M factor. The left of the plot (Zone 1) is coloured blue which represents the zone for the first type of interaction, the middle of the plot (Zone 2) is coloured green to represent the zone for the third type of interaction, and the top right (Zone 3) coloured red to represent the zone for the second type of interaction.

For the blocked slip bands that induced a stress intensity there was no obvious correlation between the M and K. However, K did tend to be smaller when the residual Burgers vector was larger assuming transfer to the best aligned prismatic slip systems. The most meaningful correlation was however between the magnitude of K and the extent of slip in the slip band (figure 5).

4. Discussion:

The slip band/grain boundary interactions in commercial purity titanium were studied with high resolution EBSD, slip trace analysis and AFM. The sample was pulled to 1% strain at low strain rate and no twinning activity was observed, therefore the observations at this stage are useful in analysing the condition for twin nucleation and the criteria for early stage slip transfer. Several blocked and transferred slip bands at randomly selected grain boundaries were studied and it was found that three categories of interactions can be observed.

The first category of interaction involves blocked slip bands leading to stress concentration in the neighbouring grain. Trace analysis shows that in each case the incoming slip band was due to dislocations on prismatic slip plane (marked red in figure 2), which agrees well with the macroscopic resolved shear stress analysis (i.e. Schmid factor). From the grain orientations (figures 2 and 4) it seems that all of the boundaries studied in this category have large rotations

between the two grains causing the basal plane normal to be close to perpendicular to each other. This generates a large misalignment of the easy slip systems. Notably in the earlier work of Britton and Wilkinson [23] the significant misalignment of slip systems was achieved with the basal planes of the two grains close to parallel but with a rotation of $\sim 30^\circ$ about the almost shared c-axis.

For this case, the stress concentration resolved onto the pile-up plane of the incoming slip band agrees well with Eshelby's model (figure 3). The stress intensity factor obtained by fitting the stress profile using equation 4 varies from boundary to boundary in the range from 0.1 MPam^{1/2} to 0.78 MPam^{1/2} with an average value of 0.41 MPam^{1/2}. The average value is in agreement with the Hall-Petch coefficient of 0.40 MPa m^{1/2} obtained by Lederich et al [16] and 0.40 MPa m^{1/2} from Armstrong et al [47] from macroscopic tensile testing of polycrystalline Ti of varying grain size. Lederich et al [16] also examined tensile deformation of CP titanium at elevated temperature of 573K, where cross slip may facilitate slip transfer and obtained a lower Hall-Petch coefficient of 0.18 MPa m^{1/2}. Salem et al [17] obtained a higher Hall-Petch coefficient of $K=0.67$ MPa m^{1/2} from room temperature compression testing of titanium, and ascribed the higher value to the increased population of twin boundaries which generated large repulsive stress on incoming dislocations and therefore provides a harder barrier for slip transfer [48]. Our stress intensity values are in broad agreement with Hall-Petch coefficient obtained from tensile testing but of course can be assessed in terms of the slip resistance offered by individual boundaries of varying geometry where stress intensities were measured.

When large numbers of dislocations have passed along the slip band to pile-up at the grain boundary the analysis of Eshelby et al [22] gives the stress intensity to be

$$\sigma'_{13}\sqrt{X} = \sqrt{\frac{N\mu b\tau}{\pi(1-\nu)}} \quad (5)$$

Where μ is the Shear modulus, ν Poisson's ratio and τ the shear stress resolved onto the slip system of the slip band. Figure 5 showed that there was a reasonable correlation between the

stress intensity factors measured by HR-EBSD and $\sqrt{N}$ estimated from AFM measurements of the slip band height. The blocked slip bands were all on slip system for which the Schmidt factor was close to 0.5 so τ is approximately half the applied tensile stress ($\tau = 115$ MPa). In every case the stress intensity measured by HR-EBSD was of the same order of magnitude but somewhat less than the value predicted from the theory of Eshelby et al [22] using the estimated number of dislocations in the slip band. This implies that there has been some relaxation of the expected stress intensity factor which could be achieved by a combination of the following mechanisms: (i) some limited slip transfer with plastic flow in a small volume of material in the neighbouring grain as seen by Britton & Wilkinson [23] and Villechaise et al [49], (ii) dissipation of some of the net Burgers vector by generation of grain boundary dislocations and their motion away from the head of the pile-up, or (iii) some cross slip across the slip band to generate a pile-up of finite width [50].

Figure 6 is an example of the slip band/grain boundary interactions which lead to slip transfer. It is not clear which slip band is the incoming one so the stress tensor is rotated onto each pile-up plane individually. As is shown in figure 6, there is no localized stress concentration induced by shear stress on the active slip plane, which indicate that slip transfer is a highly effective stress relieving mechanism. For uniformity, prismatic slip band was picked up as the incoming slip band and the other was treated as the transferred band and therefore the alignment factor M and Schmidt factor between the 'incoming' slip band and various slip systems in the neighbouring grain can be calculated. Coloured cells in table 3 indicate the pile-up plane of the transferred slip band. It can be seen that the transferred slip bands are on prismatic or $\langle a \rangle$ pyramidal slip system where the alignment is the best compared with other slip systems. For boundary 1 and 3, transferred slip systems are prismatic with almost perfect alignments with incoming slip plane while the RSS on those slip planes are small ($S_1=0.26$, 0.33 , respectively). Contrary to this, the prismatic slip system that with highest Schmidt factor ($S_2=0.5$) have the worst alignment with incoming slip plane ($M_2=0.08$ and 0.11 respectively). Figure 8 shows that the M factor effectively separates different types of interactions into their

own regions. Generally speaking, slip transfer requires both high M and S (on prismatic and <a> pyramidal system), but M is the dominant factor to consider in predicting slip transfer. Although RSS plays less important role, it is important in determining how far the transferred slip band is able to propagate, a transferred slip band is likely to terminate at a short distance from grain boundary when RSS is not enough to sustain continuous dislocation motion. Recent work using digital image correlation and EBSD by Abuzaid et al [51] showed that larger plastic strains accumulated in 'mantle' regions near grain boundaries for which slip transfer led to small residual Burgers vectors compared to those in which slip transfer was inhibited by misalignment of the predominant slip systems to give a large residual Burgers vector.

The third type of slip band/grain boundary interaction observed in this research was blocked slip bands that leads to neither stress concentration nor slip transfer. EBSD image quality map, geometrically necessary dislocation (GND) density, and σ_{13} shear stress map for two of such interactions are shown in figure 7. From figure 7 a, it can be seen that a small kink is formed at the intersection point of the slip band and the grain boundary. This kink led to a localized region of GNDs reflected back from the grain boundary into the grain containing the slip band. Neither stress concentration nor GND concentration were induced in the neighbouring grain. This is likely to be a case when stress concentration is accommodated by localised slip close to the head of the blocked slip band. By contrast figure 7 b is a case where there is no localized GND concentration but more diffuse GND distribution along the grain boundary, with again no stress concentration present around the interaction point but there seem to be a backward stress to the right of the grain boundary. In such cases it is suspected to involve absorption of lattice dislocations onto the grain boundary and the motion of grain boundary dislocations away from the head of the pile-up generating local grain boundary sliding. Figure 8 suggests that these interactions occur for intermediate values of slip system alignment. There is however considerable overlap between M factors observed for cases where a clear slip transfer occurs with the two significant slip bands intersecting at the grain boundary and M factors found for apparently blocked slip bands but where local deformation processes

have successfully relaxed the local stress concentration. A full three dimensional analysis of the boundary geometry, along with stress and dislocation density distributions below the sample surface might help resolve some of these issues.

5. Conclusion:

The High resolution EBSD technique is used to study slip band and grain boundary interactions in CP titanium deformed in tension to 1% strain. The following conclusions may be drawn:

1. At this low strain level slip band/ grain boundary interactions can be ascribed to three types: blocked slip band that induces stress concentration in the neighbouring grain, blocked slip band that does not induce stress concentration in the neighbouring grain, and slip transfer.
2. Full slip transfer requires both good alignment (high $M > 0.7$) with incoming easy slip system and high resolved shear stress on the outgoing slip system. For selecting transferred slip system, local geometric alignment seems to play a more important role than the resolved shear stress.
3. In each case of slip transfer examined HR-EBSD showed that there was no significant stress intensity associated with the intersection of the two slip bands at the grain boundary.
4. When the easy slip systems in the neighbouring grain were badly aligned with the incoming slip system to give an M factor below ~ 0.7 blocked slip bands were observed. In some such cases HR-EBSD revealed significant local stress intensity at the head of the blocked slip band but in many cases the stresses were not significant. The high stress intensity cases tend to have worse slip plane alignment.

5. Where significant local stresses were found they were broadly consistent with the 'one over square root of distance' variation expected from Eshelby et al's model [25]. The stress intensity was larger for slip bands for which AFM revealed larger plastic strains.
6. For the blocked slip bands that had no obvious stress concentrations, lattice curvature analysis indicated that GND densities were increased either in a localised feature associated with the head of the pile-up, or in a more diffuse distribution along the grain boundary. These suggest that localised plastic flow was able to relieve any stresses developed by the blocked slip band.

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