Loading and texture bias on the competitive slip activity for basal and prismatic slip systems in HCP alloys

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Abstract: Asymmetry in hexagonal crystal structure makes the occurrence of slip strongly dependent on the texture of sample. In titanium, which has a c/a ratio less than ideal, slip occurs preferentially on prismatic slip system. However other slip systems may get activated depending on the resolved shear stresses. In this paper we present results from plane strain compression experiments where the same area of the sample was imaged before and after deformation to document changes in microstructure. We then compare these results with a simple calculation of plastic strain based on activation of various slip systems depending on their respective critical resolved shear stresses. We show that incorporation of a strain rate dependent hardening parameter provides a reasonable match with the experimentally observed deformation behaviour of various grain orientations.

1. Introduction:
Titanium and its alloys high specific strength, high oxidation and corrosion resistance which makes them suitable for aerospace, biomedical and other high performance applications. Among all Ti alloys, Ti-6Al-4V (Ti64) has biggest market share. In the aerospace industry Ti64 is used largely in fuselage, nacelles, landing gear beams, fan disc, low pressure compressor discs and components of engine[1].

Ti64 is a two phase alloy with the predominant phase being α (HCP crystallite) along with a small fraction of β (BCC structure) dispersed along the grain boundaries of α phase. The α phase deforms by both slip and twinning, depending on the stress state, loading rate, and grain shape and size distribution. Of the three possible slip systems: basal, prismatic and pyramidal, prismatic is the most preferred since the c/a ratio for Ti64 is less than ideal [2–7]. In this paper we present results from plane strain compression (PSC) experiments for fine grain Ti64 samples. The average grain size was about 2 μm, thus making slip the only feasible mode of deformation[8]. Further the experiments were carried out at room temperature and at strain rates of about 10-3 s-1, both conditions favouring slip activity. So these experiments allow a detailed study of the influence of grain orientation on slip activity. The results are then compared with a simple crystal plasticity calculation for various orientations. We show that the incorporation of strain rate dependent plasticity allows us to capture the trends observed during successive deformation of near-basal and near-prismatic grains in the polycrystalline sample.

2 Experimental method
PSC was carried out using the setup shown in figure 1(a). Load is applied along the Z direction, and the sample is free to deform along the Y axis, while deformation along the X axis is restricted by the die (figure 1(b)). Figure 1c is the backscattered image of the sample before PSC showing microindent marks to identify the same area after deformation for
sequential analysis of the microstructure. Figure 1d shows the inverse pole figure map (IPF map) of undeformed sample. Grains are randomly oriented and the average grain size is about 1.9µm. It has been reported that twinning becomes more difficult with decreasing grain size and is unlikely to occur in this sample [9]. So the changes in microstructure observed after successive deformation steps can be attributed only to the slip activity in Ti64.

![Figure 1](image)

**Figure 1** (a) Set up used for PSC experiment (b) loading direction, restricted direction and free to deform direction (c) SEM image of undeformed Ti64 sample with microindent mark for imaging the same area after each deformation step (d) EBSD image of selected region.

Electron back scattered diffraction (EBSD) imaging was done for the marked region in the undeformed, 5% deformed and 7% deformed sample. From EBSD data Kernel Average Misorientation (KAM) of grain is calculated. KAM of a grain is used to quantifying the local strain accumulated in a grain due to plastic deformation [10]. In figure 2 average KAM for near basal and near prismatic (101 and 2110) oriented grains is plotted as a function of % deformation. KAM increases with deformation for all orientations, however the rate of increase is higher for near-prismatic grains as compared to the near basal grains.

It can be seen that even for the "undeformed" sample, KAM values range from about 0.5 for near-basal grains to 0.3 for near prismatic orientations.

However this spread ΔKAM decreases with increasing deformation. Since misorientation development is related to dislocation accumulation, reduction in ΔKAM is indicates less slip activity in near basal orientations relative to near prismatic oriented grains.

3. Modelling framework

In this section we present a calculation of average plastic strain in hexagonal Ti64 by calculating resolved shear stresses on all slip systems and using CRSS value as threshold for slip activation.

The resolved shear stress (τ) on the slip plane and in the slip direction is the primary driving force for slip. For each slip system α, with slip direction mα and slip plane normal nα

\[ \tau^\alpha = \sigma^c \cdot m^\alpha \otimes n^\alpha, \]  

(1)

where \( \sigma^c \) is the stress tensor in crystal coordinate system (depending on the grain orientation).

The total plastic strain tensor \( D^p \) [11] can be calculated by summation over all slip systems,

\[ D^p = \sum_\alpha \dot{\gamma}^\alpha p^\alpha, \]  

(2)

where \( p^\alpha = 0.5(m^\alpha n^\alpha \otimes n^\alpha m^\alpha) \).
Here, the shearing rate $\dot{\gamma}^\alpha$ is given by

$$\dot{\gamma}^\alpha = \dot{\gamma}^0 \left( \frac{\tau^\alpha}{\sigma'} \right)^m \text{sign}(\tau^\alpha),$$

(3)

where $\tau^\alpha = \sigma' P^\alpha$ and $\sigma'$ is the deviatoric component of applied stress tensor $\sigma$

Finally the plastic strain tensor has the form

$$D^p = \sum_\alpha \dot{\gamma}^0 \left( \frac{\tau^\alpha}{\sigma'} \right)^m \text{sign}(\tau^\alpha) P^\alpha$$

(4)

In equation 3, $\dot{\gamma}^0$ is the rate of strain in PSC experiments, taken as 0.001 sec$^{-1}$. $\sigma'$ is the critical resolved shear stress for $\alpha^\text{th}$ slip system. For titanium, CRSS values for basal, prismatic and pyramidal slip systems are in the ratio 1:0.7:3[2,12–14]. As seen from equation 3, the rate of shear depends on the strain rate sensitivity parameter, $m$, in addition to the resolved shear stress. Typically $m$ ranges from 0.01 to 0.02 for most metals [11] In our calculations, basal oriented grains show higher KAM than prismatic grains in the undeformed sample, $m$ is taken equal to 0.01 for basal and 0.005 for other orientations for 5% deformation. for next step of deformation to 7%, $m$ is 0.02 for basal and 0.018 for other orientations.

Finally from the plastic strain tensor obtained for each orientation, the effective Von Mises strain[15] can be calculated by

$$\varepsilon^p = \sqrt{\sum_{i<j} \frac{2}{3} \varepsilon^p_{ij} \varepsilon^p_{ij}},$$

(5)

4. Results and discussion

In figure 3, plastic strain due to each slip system is shown separately, along with the total effective plastic strain for $m$ values 0.005, 0.015 and 0.02. It is clear that plastic strain decreases significantly with increasing $m$. In addition, differences between various slip systems also decrease as $m$ increases.

Figure 3: The slip system wise and total effective strain with (a) $m$=0.005,(b) $m$= 0.015 and (c) $m$=0.02. (color online)

Figure 4(a) shows the effective plastic strain values calculated by using $m$ = 0.01 for basal and $m$ = 0.005 for other orientations. In our model this corresponds to 5% deformation of the specimen. The difference in the effective plastic strain between basal and prismatic orientations is 0.06. Results for 7% deformation are shown in figure 4(b) obtained by setting $m$ = 0.018 for basal and 0.02 for other orientations. These values are selected because the 5% deformed sample is expected to be more strain hardened than the starting sample, so $m$ is higher than the previous case. At the same time $\Delta$KAM is less (see figure 4(c)) so we expect less difference in the hardening response of basal and non-basal grains. The difference in the effective plastic strains obtained from this calculation for near-basal and near-prismatic orientations is 0.02.

A comparison of differences in effective plastic strain in various orientations obtained from the rate-dependent plasticity model, and $\Delta$KAM values shows that we are able to capture the trend of decreasing $\Delta$KAM with increasing % deformation. When the sample is deformed to 5%, more slip occurs in the near-prismatic grains due to a combination of orientation effect and less prior-hardening. This can be seen from calculated effective strain values and matched with the decrease in $\Delta$KAM – from 0.14 in the undeformed sample to 0.07 after 5% deformation. In the next step of deformation to 7%, both orientations are harder and
difference in effective plastic strain decreases to 0.02, while corresponding ΔKAM decreases to 0.06

![Figure 4: The total effective strain calculated for (a) first deformation step (b) for 2nd deformation step of plane strain compression (d)experimentally obtained KAM as function of deformation.](image)

5. Conclusions
- Two key observations from experiments: 1) the rate of KAM increase with increasing deformation is less for basal grains and more for prismatic; 2) spread of KAM values decreases with deformation – more deformed orientations deform less and vice versa.
- Slip activity was modeled by taking into account slip activation based on relative CRSS values for various slip system. Slip was assumed to be rate dependent. The strain rate sensitivity parameter $m$ was varied from 0.005 to 0.02 for 5% and 7% deformation.
- By selecting appropriate $m$ values depending on the KAM values of orientations, we could capture differences in the deformation response of near-basal and near-prismatic orientations, even though grain interactions have been ignored in the current model.
- Results show that the strain rate sensitivity, $m$, plays a critical role in determining the hardening response.

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