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Slip band–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 backscatter diffraction. At a low strain level, three types of interactions were observed: blocked slip band with stress concentration; slip transfer; and blocked slip band with no stress concentration. The 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 the 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 the lower critical resolved shear stress.

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 the slip band–grain boundary interaction has been cited to lead to slip transfer [2], deformation twin nucleation [3,4], cavity nucleation [5], fatigue crack nucleation [6] and a number of 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 the yield strength of a polycrystalline material to its grain size 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 rationalise it with other size effects.

The Hall–Petch coefficient has traditionally been obtained by mechanical testing of samples with varying

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grain diameter. Hyun et al. [15] have reported $k = 0.25\ \mathrm{MPam}^{0.5}$ for grade 2 commercially pure titanium (CP-Ti) deformed at room temperature under tension, while Lederich et al. [16] found $k = 0.18\ \mathrm{MPam}^{0.5}$ and $k = 0.40\ \mathrm{MPam}^{0.5}$ for pure Ti deformed under tension at 575 and 295 K, respectively. For room-temperature compression, Salem et al. [17] reported $k = 0.67\ \mathrm{MPam}^{0.5}$ for CP-Ti. Although $\sigma_y = \sigma_0 + kD_{GB}^{-1}$ has now been shown to support macromechanical 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. 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–grain boundary interaction is strongly affected by the character and structure of the grain boundaries. This suggests that boundaries with different characteristics should have different resistances 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 measured directly, while others contain parameters that depend on pre-knowledge of k, rendering those models descriptive but not predictive. The research of Bata and Pereloma [13] suggested a relatively independent model, but this suffers from difficulties of accurately determining the grain boundary strain energy and ignores stress concentrations that might arise near the grain boundary. Theoretical work by Eshelby et al. [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 Fig. 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

$$\tau = \tau_0 + \frac{K}{\sqrt{r}} \tag{1}$$

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

Britton et al. [23] recently mapped the stress distribution near the head of a blocked slip band using the high-resolution electron backscatter diffraction (HR-EBSD) technique [24,25] and found the stresses to be consistent with the Eshelby–Frank–Nabarro model. The stress intensity factor

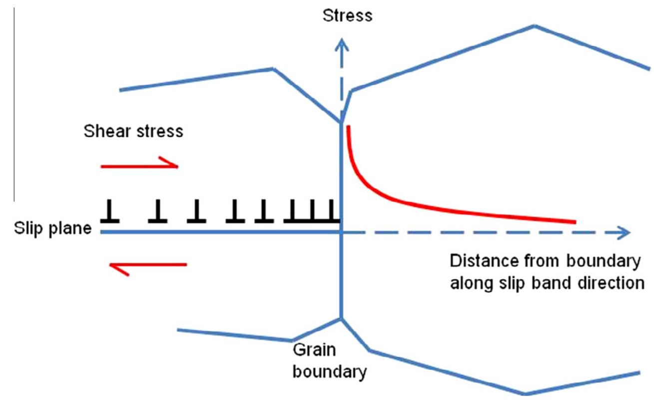

Fig. 1. Eshelby's model of dislocation pile-up at a grain boundary. The red curve to the right of the grain boundary represents the stress distribution ahead of the blocked slip band. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

K can be obtained by curve fitting 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 individually selected slip band–grain boundary interaction. It is therefore important to extend such measurement to different slip band–grain boundary interactions for the systematic evaluation of the strength of the grain boundary in terms of the alignment between crystal slip systems.

The stress concentration accumulated by the dislocation pile-up can be redistributed along the grain boundary if the Burger's vector of a grain boundary dislocation dissociated from the matrix dislocation is within the boundary plane in which it can then glide. This grain boundary gliding mechanism was described in Refs. [26,27]. If the grain boundary dislocations have a component out of the grain boundary plane, ledges can be created, which can lead in turn to the nucleation of boundary cracks [28]. This has been observed by Lee et al. [29] via an in situ transmission electron microscopy study. The most common stress relief mechanism is the generation of 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 shares a common intersection with the outgoing slip plane on the grain boundary, and the Burger's vectors of the two slip systems are equal, i.e. this transfer mechanism leaves no residual Burger's vector at the grain boundary and is akin to cross-slip for screw dislocations;
(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 the grain boundary [34]. An energy barrier proportional to the magnitude of