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Crack initiation at twin boundaries due to slip system mismatch

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What determines if a grain boundary acts as a crack initiation site during fatigue? The grain boundary defines a mismatch of slip systems, which strongly depends on the three-dimensional positions of the boundary plane. In the case of a coherent $\Sigma 3$ twin boundary, the boundary plane, and thus the mismatch between the slip systems, is known for all possible combinations of active slip systems. Thus, the tendency for crack initiation can be reduced to a purely geometric calculation.

Keywords: Twin boundaries (TB); Coherent twin boundaries (CTBs); Misorientation; CSL-$\Sigma 3$; Slip system interaction

Improving the mechanical behavior of metals and alloys by optimizing their microstructure is a major current objective of materials science. To this end, grain boundaries (GB), including their microstructural features and the resulting processes, are the main focus of so-called “grain boundary engineering” [1]. Strength, ductility and fatigue resistance may be varied by increasing or decreasing the fraction of special GBs, such as coherent twin boundaries (CTBs). The GBs are known to simultaneously improve the strength and ductility [2]. However, their influence on fatigue resistance is ambiguous because fatigue cracks often initiate at GBs, but this initiation only occurs in a small percentage of boundaries. Some studies have identified CTBs as preferred crack initiation sites that result in reduced fatigue resistance [3], while others have confirmed that CTBs offer good resistance to crack transmission and are therefore beneficial [4]. The former scenario, exemplified by damage on twin boundaries (TBs) in nickel, agrees with Neumann’s model of additional incompatibility stresses [5] and was observed by Blochwitz et al. [6]. Despite the proven strong influence of stress inhomogeneity due to the elastic anisotropy in the vicinity of GBs, several recent investigations have focused on a reduced and simple geometrical consideration of the slip systems on both sides of the boundary, as already described two decades ago [7,8]. Furthermore, the degree of accuracy with which this simple model can explain several aspects of CTB behavior is astonishing [9–11]. Finally, both the explicit computation of stress–strain incompatibilities and the reduced view of the slip system interaction originate from the crystallographic geometry as a result of the misorientation of both neighboring grains. The latter may be less advanced, but it is sufficient to explain their damaging behavior in the special case of TBs and, therefore, is more suitable for statistical calculations. Another benefit is that this reduced view works without complex 3-D finite-element simulations, making this method a simple alternative.

GBs derive their boundary character from the mismatch of the crystal lattices of neighboring grains. The well-known classification distinguishes between low-angle, high-angle and coincident site lattice (CSL)-Σ GBs. During fatigue, the movement of lattice dislocations carries local plastic deformation with boundaries that generally act as barriers [12,13]. One approach that describes this blocking effect can be derived from a purely geometric view of all orientation circumstances surrounding the boundary. To this end, the GB plane describes a discontinuity between the slip planes of neighboring grains. Furthermore, it describes a discontinuity between slip systems by considering the slip directions. However, the mismatch of the slip systems strongly depends on the 3-D position of the boundary plane. For CTBs with a misorientation of 60° along a $\langle 1\,1\,1 \rangle$-axis, the position of the boundary planes can be considered as known. The orientation of all possible slip systems in relation to the loading axis is well defined in every grain by the three Euler angles, which determine the grain orientation. Secondly, the GB can be approximated by a flat plane. In every concrete case, the active slip systems in both grains differ depending on the orientation of the grains related to the loading axis. Finally, the active slip systems in both grains and the resulting slip system combination determine if a CTB is a strong barrier to dislocation transmission and, consequently, a potential crack initiation site, or if the dislocations can pass the GB without hindrance. Therefore, the coupling of the slip systems of two neighboring grains that interact on the GB plane

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flattens to a simple mathematical three-plane cutting problem, which can be solved using analytical geometry. This method has already been performed by Lee et al. [7] and Werner and Prantl [8] during the late 1980s.

First, these workers considered the coincidence angle (α) between the intersection lines of the slip planes of the neighboring grains with the GB plane (see Fig. 1). Second, they took into account the deviation angle (β) between the slip directions. Together, both angles define the so-called transmission factor, as proposed by Clark in 1992 [14]:

$$t(\alpha, \beta) = \cos\alpha \cdot \cos\beta. \tag{1}$$

A resistance factor, similar to Blochwitz's misorientation crack factor [15], should be defined to indicate the blocking character of such a geometric misfit. The value of this factor is large when α or β, or both, are large. Because the maximum value of both angles is 90°, a logic shift can be introduced as follows:

$$\omega(\alpha, \beta) = 1 - \cos\alpha \cdot \cos\beta. \tag{2}$$

ω provides a measure to express the resistance character of the GB from a geometric point of view. A remarkable feature of ω is that the position of the GB plane strongly influences the angle α but not the angle β. Therefore, calculating $\omega(\alpha,\beta)$ for a measured misorientation is difficult because the position of the GB plane is generally not known. However, the position is known for the special case of a coherent $\Sigma3$-TB. In this case, the boundary plane is equivalent to the shared twinning plane of both neighboring crystals. Finally, all possible slip plane couplings, including their intersection behavior on the twinning plane, are symmetric and well defined by the characteristic misorientation of the twin relationship (Fig. 2). This characteristic feature of TBs related to slip transfer of dislocations was also investigated by Li et al. [11], Qu et al. [16] and Zhang et al. [9,10]. These works systematically studied the effect of the crystallographic orientation on the cracking mechanisms at TBs. Their results are based on statistical data from TB cracking compared to slip band cracking after fatigue tests. All TBs without cracks remained unconsidered. To identify the basics of the interaction between the relevant slip systems and the GBs, they defined a factor that describes the difference of the involved Schmid factors (DSF) $\Delta\Omega$ [9,10]:

$$\Delta\Omega = \Omega1 - \Omega2, \tag{3}$$

here $\Omega1$ and $\Omega2$ are the Schmid factors of the two active slip systems that interact on the GB, one in each grain. Combined with the slip morphology, they distinguish between two general cases and three subcases of different relationships between the corresponding slip planes (Fig. 2). Briefly, the DSF can be interpreted as a measure of the possibility of dislocations to slip across the GB or pile-up. As a consequence, a high DSF leads to GB cracking, while a low DSF results in slip band cracking.

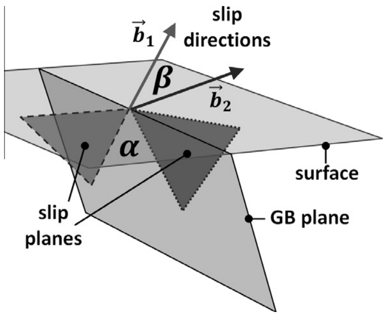

Figure 1. Visualization of the geometrical configuration of the slip systems (slip planes, slip directions) and the GB plane.

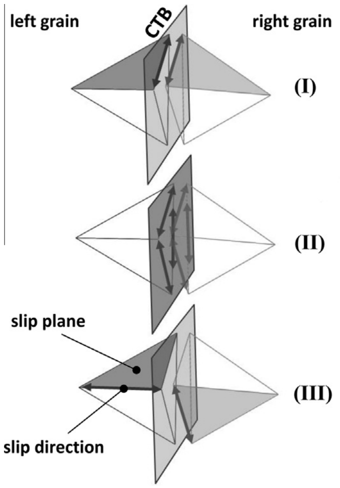

Figure 2. The three main slip system couplings taking place on a CTB: (I) cross-slip, (II) slip along the CTB and (III) blocked slip as consequence of mismatching slip systems.

In this work, different characteristic cases are identified to explain crack initiation at CTBs. This identification leads to a prediction of the sites with an increased crack initiation probability in polycrystalline specimens. The current approach is based on the prioritization of the geometric correlation between interacting slip systems. Additionally, it also considers the Schmid factor distribution, which determines the effective slip system activity. Therefore, all of the $12 \times 12 = 144$ possible face-centered cubic–slip system interactions must be quantified by their particular angles, α and β, for two neighboring grains. The basic types of slip system couplings exist for the CTBs with default values of $\alpha = 0°$, $60°$ and $\beta = 0°$, $34°$, $60°$, $71.5°$ and $90°$, as shown in Figure 2:

(I) Cross-slip: a symmetric pair of slip planes, one in each grain, coincides on the TB. Hence, $\alpha = 0°$, and if β is also equal to $0°$, the common slip direction is active. Therefore, all requirements for cross-slip are fulfilled. Consequently, $\omega = 0$ and the (geometric) resistance effect is absent.

(II) Slip along the TB: if the active slip is limited to the shared TB plane, a pseudo-coupling or self-coupling of two equal slip planes occurs. This coupling results in a vanishing geometric GB resistance and an unimpeded slipping process.

(III) Blocked slip: a non-symmetric pair of slip planes interacts in the TB plane. Hence, α and β become large and a distinctive resistance, ω, consequently develops. For example, this value is defined as follows for the concrete numerical value from Figure 1:

$$\omega(\alpha, \beta) = 1 - \cos 60° \cdot \cos 71.5° = 0.84. \tag{4}$$

The three different slip system couplings from Figure 2 provide a full description for even more complex cases of coupling with the superposition of different active slip systems in one or both grains.