

Title:

FATIGUE CRACK NUCLEATION IN METALLIC MATERIALS

CONF-981216--

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Submitted to:

Small Fatigue Cracks: Mechanics of Mechanisms,  
Oahu, HI, 12/6-10/98

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## FATIGUE CRACK NUCLEATION IN METALLIC MATERIALS.

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### ABSTRACT

The process of fatigue crack nucleation in metallic materials is reviewed placing emphasis in results derived for pure FCC metals with wavy slip behavior. The relationship between Persistent Slip Bands (PSB's) and crack initiation will be examined for both single crystals and polycrystals, including the conditions for inter- and transgranular crack nucleation and their connection to type of loading, crystallography and slip geometry. The latter has been found to be an important parameter in the nucleation of intergranular cracks in polycrystals subjected to high strain fatigue, whereby primary slip bands with long slip lengths impinging on a grain boundary produce intergranular crack nucleation under the right conditions. Recent results related to intergranular crack nucleation in copper bicrystals and crack nucleation in Cu/Sapphire interfaces indicate that this mechanism controls crack nucleation in those simpler systems as well. Furthermore, it is found that under multiple slip conditions the crack nucleation location is controlled by the presence of local single slip conditions and long slip lengths for a particular Burgers vector that does not have to be in the primary slip system.

**KEYWORDS:** fatigue, cyclic deformation, crack nucleation, persistent slip bands, strain localization, slip geometry.

### INTRODUCTION

Fatigue crack initiation is an issue of extreme scientific importance, since our quantitative understanding of the basic process behind it is far from complete [1], and also a challenging technological problem, as small smooth components in critical applications can experience short fatigue lives after cracks nucleate, depending on the dimensions of the component and the properties of the material.

The stage within the fatigue life at which a crack initiates is defined to a great extent by the determination of the investigator and the techniques used to find the incipient cracks. The locations for crack nucleation, on the other hand, have been well established to be associated with microstructural features that produce either stress concentrations or strain localization, such as PSB's, grain boundaries, inclusions, etc.

The mechanisms that control fatigue crack nucleation and some of the models used to describe them will be briefly reviewed in this paper. Given the large amount of literature and results available in the subject, the scope of the article will be limited to initiation mechanisms that arise purely from the deformation process in FCC metals with wavy slip characteristics. Emphasis will be placed on the roles of dislocation arrangements and microstructure, in both mono- and polycrystalline materials. The role of PSB's in fatigue crack nucleation will be explored. The connection between PSB's, loading type and intergranular crack nucleation will also be established. Furthermore, recent results obtained in Cu bicrystals and Cu/Sapphire samples will be used to illustrate the effects of slip geometry and crystallography in intergranular/interfacial fatigue crack nucleation in notched samples tested under high cycle fatigue conditions.

## FATIGUE CRACK NUCLEATION IN CU SINGLE CRYSTALS.

Fatigue crack initiation in Cu single crystals, and many FCC materials, is closely related to the development of surface roughness, which in turn results from the onset and growth of zones of strain localization, i.e., PSB's in wavy slip metals and Persistent Lüders Bands (PLB's) in planar slip. Ma and Laird [2] showed that, in Cu single crystals tested under strain control, fatigue cracks tend to nucleate preferentially at the leading edge of the intersection of a PSB with a positive protrusion and the surface of the sample, as can be seen in Fig. 1.



Fig. 1. Stage I fatigue crack at the leading edge of a macro-PSB in a Cu single crystal tested for 60,000 cycles at a strain amplitude of  $2 \times 10^{-3}$ . After Ma and Laird [2].

The origin of these fatigue cracks has been often explained in terms of a model first proposed by Wood [3]. The idea behind this model is that the repeated cycling of the material results in different amounts of net slip on different glide planes and the shear displacements along the slip bands then become irreversible. This irreversibility results in surface roughening and the gradual development of a "hill-and-valley" configuration [1, 4]. The valleys present in the new rough surface act as micro-notches promoting additional slip. This is likely to be more pronounced in tension, since the micro-notches can close in compression reducing the stress concentration, which further enhances irreversibility of slip [1]. An outline of this mechanism is shown in Fig. 2.

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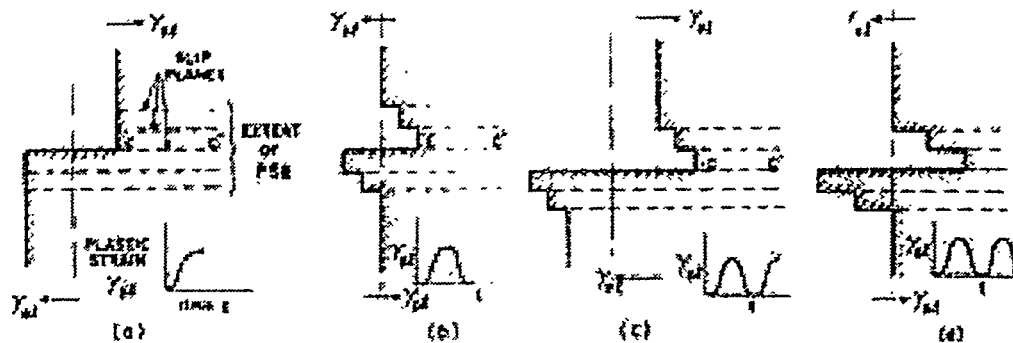


Fig. 2. Outline of surface roughening mechanism in a PSB, after the initial slip step at the surface produced in tension, as shown in (a). Note that the loading sequence is given by the inserted  $\gamma_{pl}$  vs. time plot. After Laird [1].

Note from Fig. 2 that, during compression, cycles (b) and (d), the strain is more uniformly distributed on the slip planes, which are shown as dotted lines. The irreversibility of slip from (a) to (d) finally results in a deep valley that will eventually become a crack. This mechanism can explain the formation of intrusions and extrusions. Formation of protrusions in macro-PSB's, on the other hand, have been attributed to swelling of the material due to vacancy generation inside the band during cycling [1]. Some of the mechanisms for vacancy generation have been linked to fatigue crack nucleation via vacancy-dipole models. A prime example of these models is the one proposed by Essmann *et al* [5]. According to this model, the preferential annihilation of vacancy-type dipoles inside a slip band will eventually result in slip irreversibilities that give origin to a series of edge dislocations at the PSB-matrix interface, which put the slip band in compression. It is assumed that these dislocations are able to glide to the surface, thereby producing surface roughness in the direction of the slip vector.

The presence of edge dislocations at the PSB-matrix interface has the advantage of being amenable to modeling using continuum mechanic approaches. This has resulted in the formulation of fatigue crack initiation models based on the accumulation of elastic strain energy due to the presence of these edge dislocations, e.g., the model proposed by Mura and Nakasone [6]. A disadvantage of these models is that they are in conflict with the well known phenomenon of reduction of elastic energy that seems to govern the development of dislocation structures under cyclic loading [1]. Another model based on vacancy generation was published by Repetto and Ortiz [7]. In this model, the diffusion of vacancies produces a groove at the PSB-matrix interface that eventually sharpens to form a crack. Some of these models have been used to explain fatigue crack nucleation phenomena in polycrystals, as will be discussed in the next section.

## FATIGUE CRACK NUCLEATION IN CU POLYCRYSTALS.

Fatigue cracks have been shown to nucleate intergranularly in polycrystals tested at strain amplitudes higher than those required to produce PSB's. At these levels of strain,  $1 \times 10^{-3}$  or more, the dislocation structure consists of dipolar walls or complex cell structures and the deformation is highly homogeneous throughout the specimen, promoting grain boundary cracking. Kim and Laird [8] noted that this crack nucleation was preceded by the formation of a slip step at a grain boundary that gives rise to a notch and, eventually, to a crack. They found that certain boundaries were more susceptible to crack nucleation, as long as they satisfy the following conditions:

- a) The two grains at each side of the boundary are highly misoriented.

b) The active slip system of at least one grain is directed over large distances at the intersection of the boundary with surface of the specimen.

Figure 3 shows an example of the formation of intergranular crack initiation sites at the intersection of primary slip bands and a grain boundary in a Cu polycrystal cycled under plastic strain control at an amplitude of  $2 \times 10^{-3}$ . The process is portrayed at two different levels of accumulated plastic strain, as reported by Figueroa and Laird [9]. Nucleation sites are indicated by arrows. They also reported that, at lower strain amplitudes,  $1 \times 10^{-4}$  or so, the crack nucleation sites in polycrystalline copper tested under strain control were also dominated by grain boundaries, with some cracks nucleating and growing along PSB's.

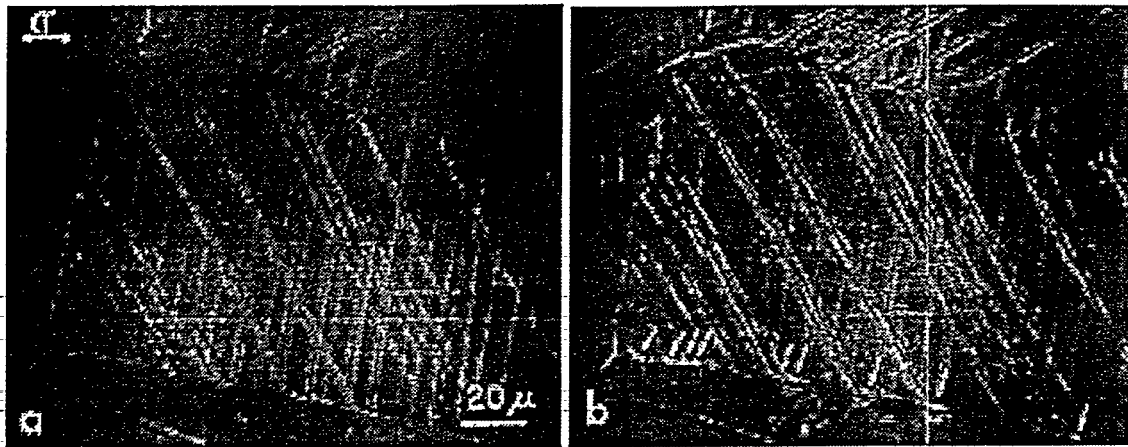


Fig. 3. Intergranular crack initiation (a) Sample at a cumulative plastic strain of 12; (b) Sample at a cumulative plastic strain of 28. After Figueroa and Laird [9].

The effect of different loading modes on crack nucleation in Cu polycrystals was investigated by Ma, Laird and Radin [10], who studied the influence of ramp loading in life and failure mode. These investigators found that ramp loading extends the life of the samples and changes the dominant failure mode from intergranular to transgranular. This occurs if the stress or strain amplitude is not high enough to transform PSB's in the bulk of the grains to dislocation cells. An example of dominating transgranular fracture in a Cu polycrystal tested at 88 MPa after ramp loading to 98 MPa is shown in Fig. 4.



Fig. 4. Transgranular stage I cracks in a polycrystalline copper specimen. After Ma, Laird and Radin [10].

The experimental observation of intergranular fracture at PSB-boundary intersections have stimulated the use of dislocation pile-up models to explain crack nucleation. The models are

based on the presence of edge dislocations at the PSB-matrix interface predicted by the mechanism proposed by Essmann *et al* [5]. An outline of this model is shown in Fig. 5.

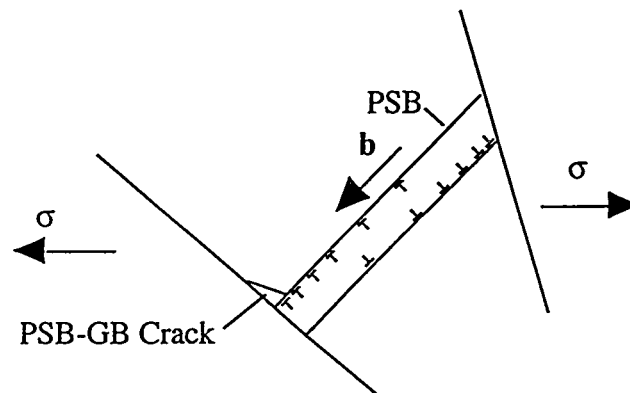


Fig. 5. Formation of a PSB-Grain boundary crack due to a pile-up of interface edge dislocations. After Liu *et al* [11].

This model has been treated and extended several times in the literature [6, 11-14]. Note that a problem with this model is that the effect of the stresses produced by the pile-up is assumed to be directly involved with fracture, and the possibility of shielding and relaxation of the stresses due to plastic deformation in the adjacent grains has not been addressed. Laird [1] has also indicated that the presence of a free surface is required to produce a notch in the grain boundary that can eventually result in a crack, since in the bulk of the sample the constraint of the matrix would preclude it [4].

Annealing twin boundaries in FCC materials are also well known sites for fatigue crack nucleation, despite their being low energy interfaces [4, 15]. This has been related to the fact that PSB's often appear next to (111) twin boundaries [16], which in turn is due to local stresses that arise due to strain compatibility requirements [15, 17]. It has also been found that in a stack of twins, cracks nucleate every other boundary. This was explained by Neumann and Tönnessen [18], by noting that the superposition of the compatibility stresses at the twin boundaries and the applied stresses favor slip only every other boundary. Fatigue crack nucleation will be discussed in the next section for high angle boundaries located close to a notch in samples tested under low strain conditions, using recent results obtained in Cu bicrystals.

## FATIGUE CRACK NUCLEATION IN CU BICRYSTALS.

An effective technique to study and isolate grain boundary effects during cyclic deformation is via the use of bicrystal specimens. Pure copper bicrystals were prepared for this goal by diffusion bonding with the crystallography shown in Fig. 6.



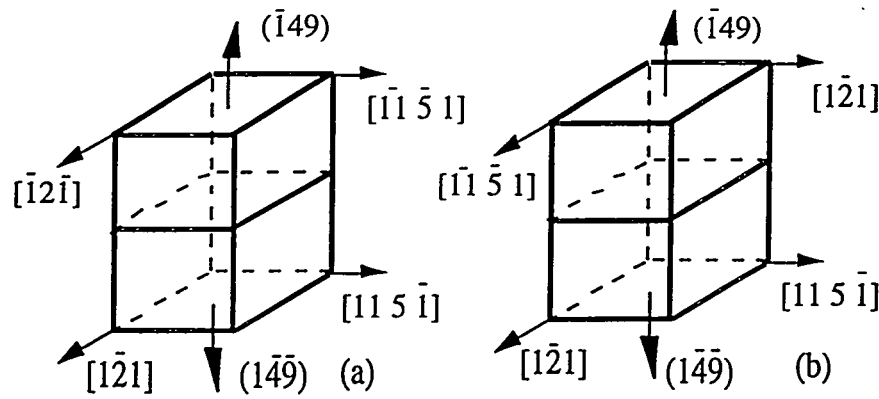


Fig. 6. Crystallography of Cu bicrystals used for testing. (a) 180° Twist boundary about  $[1\bar{4}9]$ ; (b) 90° twist boundary.

The bicrystals were first cycled to saturation at a plastic strain amplitude of  $5 \times 10^{-4}$  to establish a dislocation structure uniformly, i.e., without the effects of stress concentrations other than that of the boundary. The test was then stopped and a small notch ( $K_f \approx 3$ ) was spark-machined at one edge in the plane of the boundary. The material affected by spark-cutting was removed by a light electropolish and the test restarted. Cracking behavior, initiated at this notch in the direction chosen for study regarding the slip geometry, was observed by *in-situ* optical microscopy. The notch positions used for each misorientation are shown in Fig. 7, in relation to the traces of the primary slip planes in the two grains.

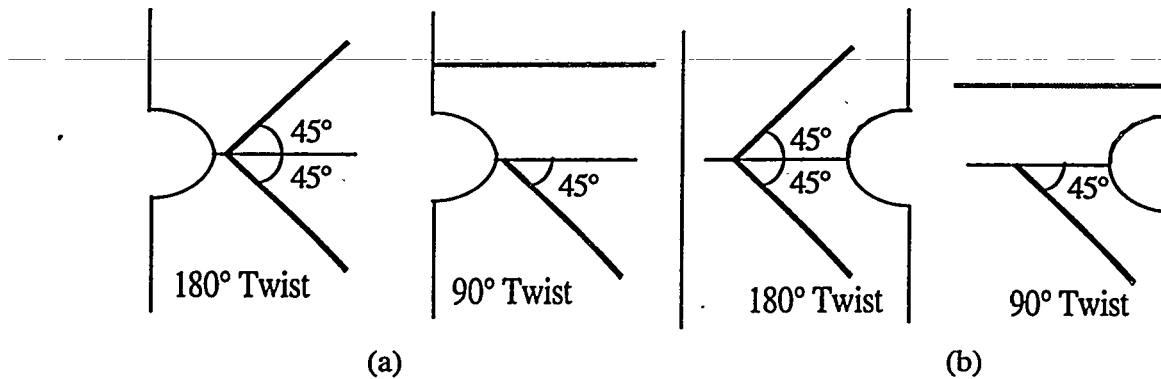


Fig. 7. Position of the notch with respect to the primary slip plane trace in each grain for the two misorientations tested. (a) "Favorable" configuration; (b) "Unfavorable" configuration.

The term "favorable" in Fig. 7 refers to slip geometries ahead of the expected crack that favor forward slip at the crack tip, which is known to favor fatigue crack propagation [19]. Propagating cracks nucleated from the notches could be readily detected, since they produced a distinct zone of multiple slip. Once a crack was detected, its nucleation location was established and the test was continued. The results presented here pertain to the relationship between the nucleation site and the slip geometry of the samples.

The four samples with 180° twist boundaries that were tested with "favorable" notch configurations all had a crack nucleating at the same location, i.e., the intersection between one of the side surfaces, the notch and the grain boundary. A micrograph of the crack nucleation site is shown in Fig. 8.

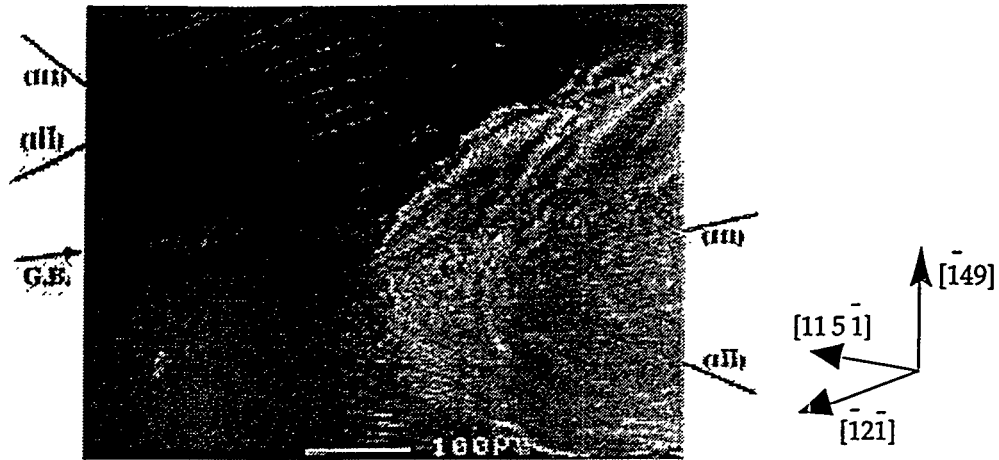


Fig. 8. Crack nucleation site for a 180° twist boundary with a "favorable" notch. The specimen has been tilted inside the SEM to observe two sides of the notch simultaneously.

The sample was tilted almost 45° inside the SEM in order to observe two sides of the notch at the same time. One of the edges of the sample faced the electron beam, in this case the edge between the  $-(11\ 5\ \bar{1})$  and  $(\bar{1}\ 2\ \bar{1})$  planes of the lower grain of the sample. Note how the primary slip plane, (111), has a long slip length ahead of the nucleation site, whereas the critical slip plane,  $(1\ \bar{1}\ \bar{1})$ , has a long slip length towards the right hand side of the nucleation site. An outline of the slip geometry in the lower grain is shown in Fig. 9.

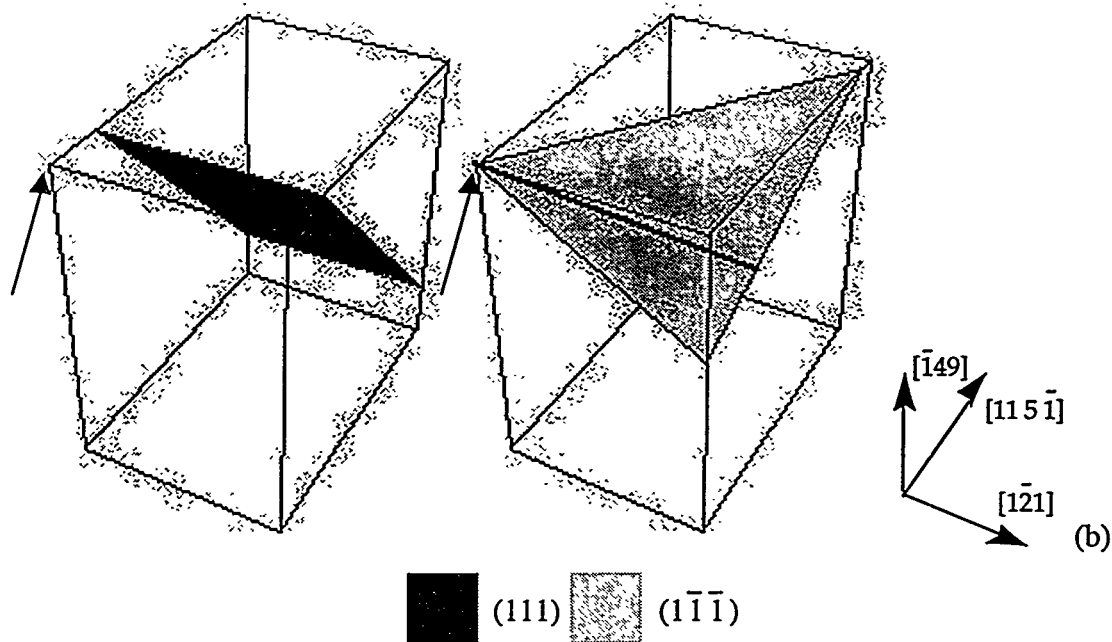


Fig. 9. Slip geometry for the lower grain. The crack nucleation site is marked by arrows. The thick line indicates the slip length of the  $[01\ \bar{1}]$  Burgers vector.

Note that the primary Burgers vector for the tensile axis used,  $[\bar{1}01]$ , is contained on the  $(\bar{1}21)$  face, and points directly towards the point of crack nucleation. The Burgers vectors with the second and third highest Schmid factors have zero slip length at both corners of the face of the crystal where the notch was located; however, the slip vector with the fourth highest Schmid factor (0.29),  $[01\ \bar{1}]$  in this case, has a relatively long slip length towards the nucleation site, as shown in the figure. The situation in the upper grain is identical, as far as the slip lengths

towards the same corner <sup>are</sup> is concerned, since the boundary is a mirror plane for this misorientation.

Cracks in samples with 90° twist boundaries nucleated at the same position with respect to the lower grain, which is common to both misorientations (see Fig. 6). In this case, the primary slip vector in the upper grain also points towards the nucleation site. It seemed that the Burgers vector with the largest slip length and a significant Schmid factor was the element that decided the location of the nucleation site.

Samples with the same misorientation but “unfavorable” notches also shared a common nucleation site for all tests. A micrograph of the nucleation site for this case is shown in Fig. 10. The sample was also tilted about 45° inside the SEM in order to observe two sides of the notch at the same time. One of the edges of the sample faced the electron beam, in this case the edge between the  $(11\bar{5}\bar{1})$  and  $(\bar{1}2\bar{1})$  planes of the lower grain of the sample. An outline of the nucleation site and the slip geometry in the lower grain of the sample is shown in Fig. 11.

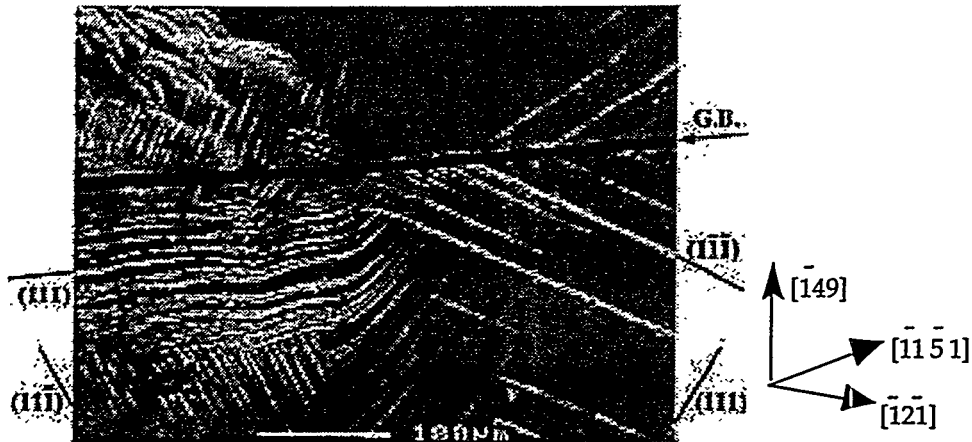


Fig. 10. Crack nucleation site for a 180° twist boundary with an “unfavorable” notch. The specimen has been tilted inside the SEM to observe two sides of the notch simultaneously.

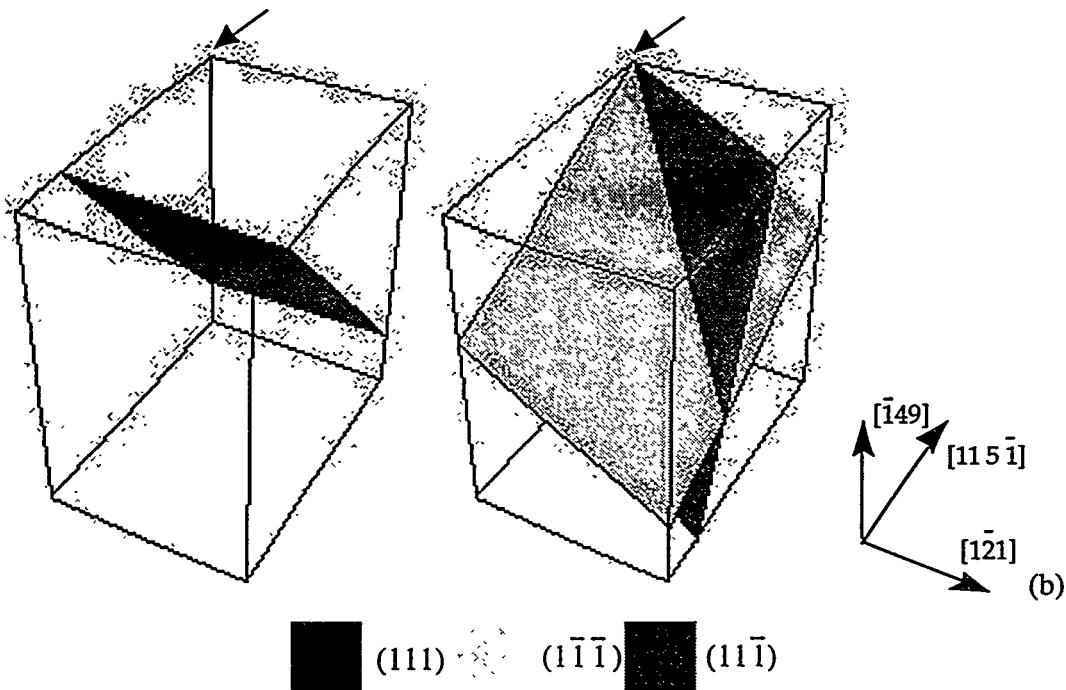


Fig. 11. Slip geometry at the notch for the lower grain. The nucleation site is marked by arrows. The intersection of  $(1\bar{1}\bar{1})$  and  $(11\bar{1})$  is the  $[101]$  Burgers vector.

The slip length of the primary slip system is zero at the nucleation site for this sample; however, the slip vector with the second highest Schmid factor (0.47),  $[10\bar{1}]$ , had a significant slip length towards the site of nucleation. This direction is common to both the critical  $(1\bar{1}\bar{1})$  and the conjugate  $(11\bar{1})$  slip planes, as shown in Fig. 11. Samples with  $90^\circ$  twist boundaries and “unfavorable” notches also had their nucleation sites located at this particular corner. Note that, for this misorientation, the primary slip vector in the upper grain can also contribute, since it has a long slip length towards the nucleation site. This evidence seems to support the mechanism proposed by Kim and Laird [8], since nucleation took place at locations where slip systems with long slip lengths were pointed towards the intersection between the boundary and the surface, only that in this case the particular slip vectors were not always in the primary slip system, as the notch produced local multiple slip conditions. The application of this mechanism seems to extend to metal/oxides interfaces, as will be discussed in the next section.

## FATIGUE CRACK NUCLEATION IN CU/SAPPHIRE BICRYSTALS.

Peralta and coworkers [20], have reported observations on the nucleation of interfacial fatigue cracks in cylindrical Cu/sapphire bicrystals. The samples were prepared by diffusion bonding under ultra-high vacuum conditions [21]. The geometry and crystallography of the bicrystals are shown in Fig. 12.

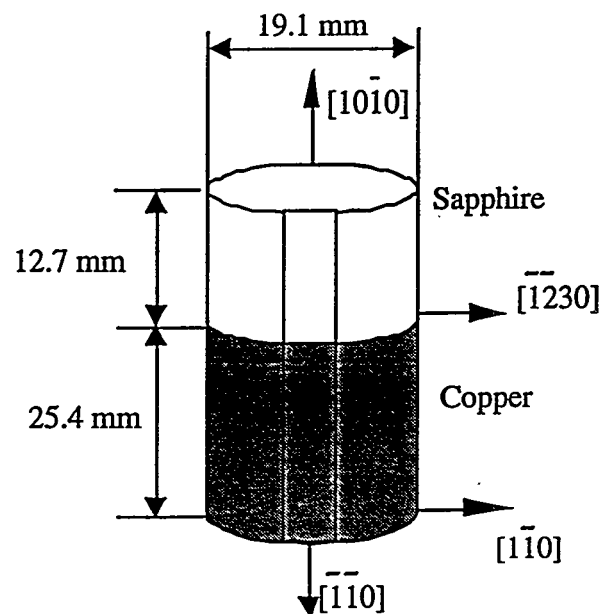


Fig. 12. Geometry and crystallography of the Cu/Sapphire bicrystals. After Peralta *et al* [20].

A circumferential notch was machined at the interface and the samples were tested under compression-compression loading perpendicular to the interface. Tests were started at an initial stress amplitude  $\Delta\sigma = 20$  MPa, which was increased by 5 MPa increments and tests were continued. Crack growth was first observed at a stress amplitude of 40 MPa after 6,000 cycles. Three initiation sites were observed located at  $\sim 125^\circ$ ,  $216^\circ$  and  $-55^\circ$  from the x-axis, which was chosen parallel to  $[001]$ . A schematic is outlined in Fig. 13. A picture showing the thumbnail crack that developed from the nucleation site at  $-55^\circ$  can be seen in Fig. 14, as was observed on the Cu fracture surface once the sample was broken.

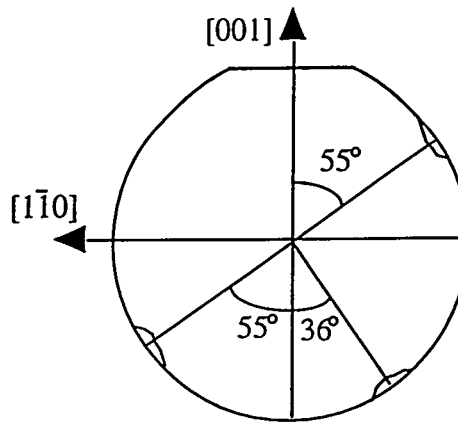


Fig. 13. Outline of the positions of initial crack nucleation sites. After Peralta *et al* [20].

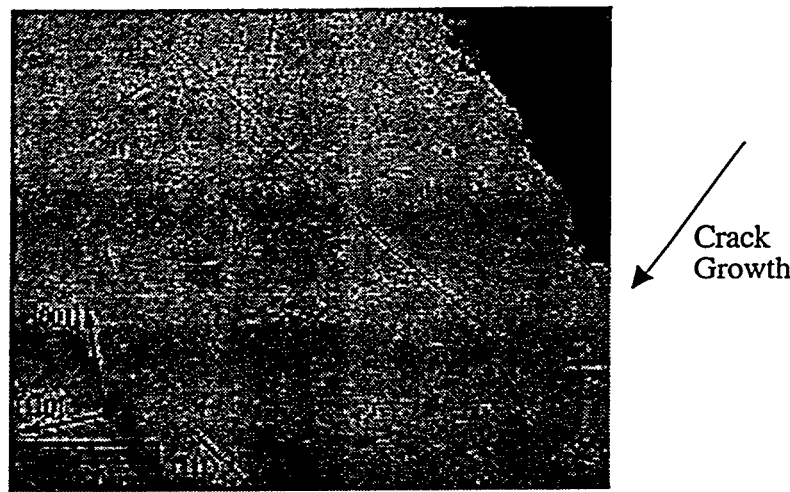


Fig. 14. Nucleation site at  $-55^\circ$  from  $[001]$  on the Cu fracture surface. After Peralta *et al* [20].

Note that the front of this thumbnail crack is parallel to the trace of the  $(1\bar{1}\bar{1})$  slip plane on the  $(110)$  plane of Cu. The uniformly spaced markings in front of the thick line where the crack first arrested suggest that propagation took place along a direction perpendicular to the  $(1\bar{1}\bar{1})$  slip trace, with the crack front parallel to that trace.

It can be argued there should have been four crack nucleation sites, by symmetry. It is suspected that the absence of crack initiation at the first quadrant of the interface plane (see Fig. 13) has to be related to irregularities in the notch geometry and deviations resulting from the alignment of the single crystal and the testing setup rather than an intrinsic crystallographic mechanism. Given the well-defined locations of the nucleation sites it is quite possible that there exists a correlation between the position of these sites and the slip geometry on the Cu side, similar to that suggested by Kim and Laird [8]. The slip length was plotted for the four slip systems with the highest Schmid factors (S.F.) in a Cu single crystal with a  $[110]$  loading axis:  $(111)[10\bar{1}]$ ,  $(111)[01\bar{1}]$ ,  $(11\bar{1})[101]$ , and  $(11\bar{1})[011]$  (all with S.F.=0.408).

The resulting slip length as a function of the angle  $\theta$ , which defines the position on the perimeter of the cross section, is shown in Fig. 15 for the four slip vectors studied.

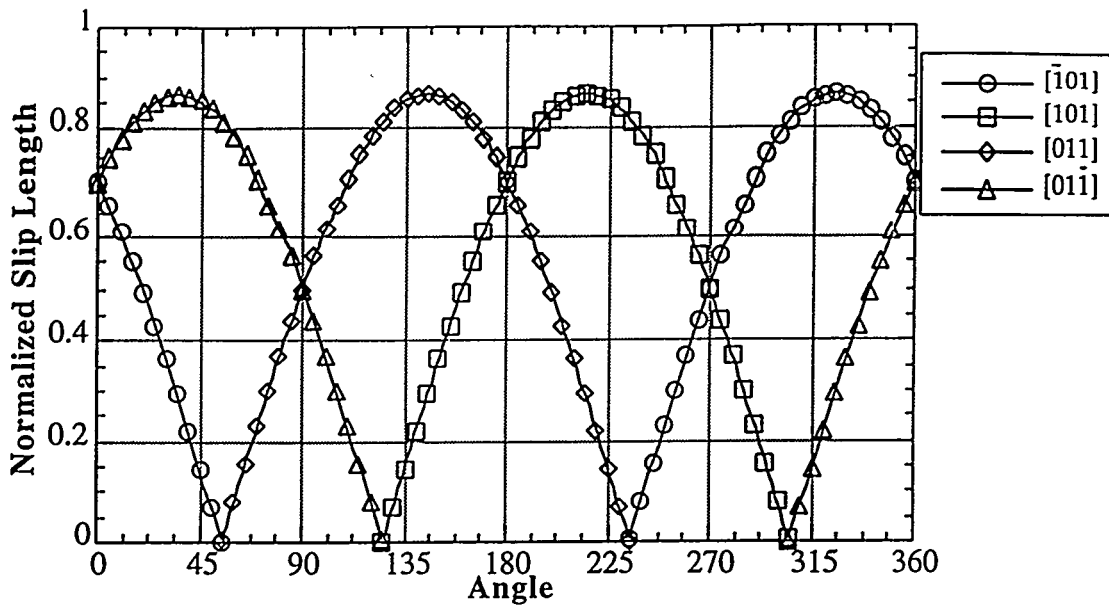


Fig. 15. Normalized slip length for four Burgers vectors. After Peralta *et al* [20].

Note that the angles for maximum slip length are located at 35.26°, 144.74°, 215.26° and 324.74° from [001]. The third location is in good agreement with the position of the crack nucleation site in the third quadrant (216°). The sites at -55° (305°) and 125° do not coincide with the positions of maximum slip length for the corresponding slip vectors. However, note from Fig. 13 that points located at these angles are also significant: they correspond to positions where only one Burgers vector has a slip length different from zero, i.e., there is a local single slip condition for these angles. Note also that for all slip vectors considered there is some overlapping between the vector with the maximum slip length and the vector with the second longest length for some angular range. This second component is one third of the maximum slip length for the angle where the maximum is located. The value of slip length for the angle where only one Burgers vector has a slip length different from zero is about 94.3% of the maximum. This suggests that strong single slip might be necessary to induce crack nucleation due to the impingement of slip bands at the interface, since the presence of another Burgers vector may affect the process leading to crack nucleation. The fact that one of the nucleation sites coincides more or less exactly with the point of maximum slip length and that one quadrant did not have cracks at all, points out to a lack of homogeneous multiple slip in the sample. Inhomogeneous distribution of slip in fatigue of copper single crystals oriented for multiple slip has been observed [22] and it is usually related to misalignments during preparation and testing of the samples. Nevertheless, the fact that a correlation could be established between the location of the nucleation sites and the slip geometry indicates that crack nucleation at the interface is controlled by the slip process in the Cu side.

## CONCLUSIONS

Fatigue crack nucleation in Cu single crystals is controlled by the irreversibility of slip within PSB's, which manifests itself through the formation of surface roughness. This surface roughness eventually produces a sharp crack, usually at the PSB-matrix interface.

Fatigue crack nucleation in Cu polycrystals is intergranular when conventional loading methods are applied and slip bands point towards the intersection of the grain boundary and the surface of the sample with a long slip length, or when the amplitude of strain is high enough to produce cell structures. Changing the initiation of the test to ramp loading can promote

transgranular fracture along PSB's as long as the amplitude of the loads is low enough to prevent the formation of cells.

Tests carried out in pure Cu and Cu/Sapphire bicrystals have provided evidence that fatigue crack nucleation in notched samples tested under high cycle fatigue conditions is also controlled by the slip geometry via slip bands with long slip lengths directed towards the intersection of the interface and the surface of the sample. The slip vector that promotes crack nucleation was not always in the primary slip system.

## ACKNOWLEDGMENTS

This work was supported by the Department of Energy, Office of Basic Energy Science, a postdoctoral fellowship to P. Peralta at Los Alamos National Laboratory and a start-up grant to P. Peralta from Arizona State University. This support is greatly appreciated. P. Peralta also thanks the Engineering Foundation for awarding him a grant to attend this conference.

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