Final Performance Report

MICROSTRUCTURE AND 3-D EFFECTS IN FRETTING FATIGUE OF TI ALLOYS AND NI-BASE SUPERALLOYS

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Summary
Fretting fatigue is often the root cause of nucleation of high cycle fatigue (HCF) cracks in clamped components. Damage and plastic deformation accumulation in fretting fatigue occurs within a depth of a few crystallographic grains. Therefore, more accurate assumptions concerning length scale, damage volume, and the material model are needed to establish a more solid physical foundation necessary for next generation fretting fatigue damage prediction. Major thrusts include: (1) development and implementation of a 3-D crystal viscoplasticity model for Ti-6Al-4V, (2) realistic 3-D fretting simulations that capture influence of key microstructure features, including distinct phase properties and crystallographic texture, and (3) experimental characterization of fretting experiments to both validate fretting simulation results and identify additional features to incorporate in the crystal viscoplasticity model and fretting simulations.

A 3-D crystal viscoplasticity model of duplex Ti-6Al-4V has been developed that is capable of representing arbitrary crystallographic textures, the unique crystallography of the constituent phases, anisotropy of slip system strengths, and non-planar dislocation core structures. These features are essential to capturing the deformation behavior of these materials due to the low symmetry of the hcp crystal structure and the resulting anisotropic properties. These material models are coded in FORTRAN as ABAQUS User MATerial subroutines.

Fretting contacts are simulated by finite element analysis. The simulations are carried out for several microstructural realizations with emphasis placed on understanding how texture and tangential load affect the fatigue life. The results clearly demonstrate the importance of the various sources of microstructural heterogeneity in the surface layers. The main sources of microstructural heterogeneity include the distribution of phases, slip system strength anisotropy, and crystallographic texture.

Automated electron backscatter diffraction (EBSD) is used to establish how fretting spatially evolves microtexture and the relationship between crystallographic orientation, grain boundaries and formation of subgrains and cracks in the fretting process volume. It is a useful tool to quantify evolution of strain-induced microstructural changes due to deformation in the near-surface layers. To establish the role of crystallographic orientation on the fretting damage response, a fretting study on single crystal Ni-base superalloy, PWA 1484, was conducted. The orientation dependence in fretting is primarily associated with the orientation dependence of plastic deformation in the near surface material. Hence, crystal plasticity and relevant lower microstructure length scale models are necessary to predict these observations.

Research Objectives

- To develop a microstructure-based fretting crack formation prediction methodology that incorporates microstructure heterogeneity and a more realistic treatment of crystallographic slip using crystal plasticity models, necessitating development of crystal plasticity models for hexagonal closed-packed (HCP) materials with focus on Ti alloys and the identification of new fatigue indicator parameters.
- To develop realistic 3-D crystal plasticity models for Ti-6Al-4V that include the influence of multiple phases, phase distributions, and the shear enhancement associated with the highly heterogeneous deformation field.
- To validate the modeling approach by comparing simulations to observations of degradation in fretting experiments conducted on Ti-6Al-4V as well as a single crystal Ni-base superalloy.
- To evaluate fretting maps that indicate the character of the cumulative plastic strain and fretting degradation utilizing fully 3-D crystal plasticity.

Accomplishments and Innovations

Development of 3-D crystal plasticity models for Ti-6Al-4V

A 3-D crystal plasticity model for $\alpha+\beta$ Ti-6Al-4V with duplex microstructure has been developed (Mayeur, 2004; Mayeur and McDowell, 2007). The microstructure consists of a primary α-phase which is of hcp crystal structure and a secondary lamellar ($\alpha+\beta$) phase which is comprised of alternating lamellae of secondary α-phase and bcc-structured β-phase. A 2-D crystal plasticity model of duplex Ti-6Al-4V developed in a prior AFOSR-sponsored project (F49620-01-1-0034) employed a planar triple slip idealization (Goh et al., 2006a and references therein). This prior study was a pioneering effort to show effect of grain orientation distribution, grain size and geometry, as well as the phase distribution and their arrangement in fretting contact problems, suggesting that the role of micro-textures (and indeed primary α size and orientation) might be significant in resisting fretting fatigue (Goh et al., 2006b). The 3-D model developed in this project is capable of representing arbitrary crystallographic textures, the unique crystallography of the constituent phases, anisotropy of slip system strengths, and non-planar dislocation core structures. These features are essential to capturing the deformation behavior of these materials due to the low symmetry of the hcp crystal structure and the resulting anisotropic properties.

The model includes the 24 active slip systems in the primary α-phase (Figure 1): 3 basal, 3 prismatic, 6 first-order pyramidal with <a> slip vector, and 12 first-order pyramidal with <c+a> slip vector. The <c+a> slip systems are necessary to accommodate deformation along the c-axis as the basal, prismatic, and first-order pyramidal <a> slip systems do not comprise a set of five linearly independent slip systems that fulfill requirements for representing arbitrary inelastic deformation rates. The relative magnitudes of the critical resolved shear stress

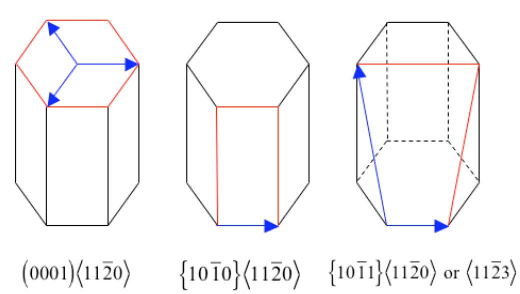

Figure 1. Slip systems in the primary α-phase.

(CRSS) are ordered as $\tau_{prism} \le \tau_{basal} < \tau_{pyr<a>} < \tau_{pyr<c+a>}$. The dislocation core model of Naka et al. (*Phil. Mag. A*, Vol. 57, 1988) is included to capture the non-Schmid behavior in the α phase due to dislocation dissociation from the prismatic plane onto two first-order pyramidal planes.

The individual phases in the lamellae (α+β) grains are not explicitly represented in this model as this would be prohibitive in a polycrystal simulation. Instead, the lamellae (α+β) grains are represented implicitly by including both hcp and bcc slip systems aligned according to the Burgers orientation relationship (BOR). These implicit (α+β) grains also have 24 slip systems: 3 basal, 3 prismatic, 6 first-order pyramidal <a>, and 12 (110) $\langle 111 \rangle$ bcc slip systems. It is believed that these lamellar regions, and more specifically the α/β interfaces, are responsible for improved fatigue properties. According to the BOR the basal planes of the secondary α-phase are parallel to one of the (110) planes of the β-phase. Additionally, one of the prismatic planes is nearly parallel to the interface plane. It is assumed that these slip systems are more easily activated and/or transmitted through the lamellar colony, and the remaining slip systems are significantly harder to activate and/or transmit due to the relative crystallographic misalignment and reduced slip length. A Hall-Petch type of relation is employed as a contribution to slip system strength based on mean free path for dislocations on different slip systems in each phase. These material models are coded in FORTRAN as ABAQUS User MATerial subroutines.

As part of the model development, a series of parametric studies simulating uniaxial deformation were designed to determine the sensitivity of the macroscopic yield stress (for a randomly textured polycrystal composed entirely of primary α-phase) on the relative ratios of the CRSS for the different slip families (Mayeur and McDowell, 2007). Polycrystal simulations reproduce the dependence of the elastic modulus and macroscopic yield strength on texture. These simulations also show the desired result that the majority of the plastic deformation is contained within the contiguous regions of the primary α-phase, also consistent with experimental observations. Consideration of more realistic microstructure morphologies using Voronoi tessellation coupled with simulated annealing techniques have also been considered (Zhang et al., 2007; Zhang, 2008).

It is well known that fatigue crack formation within Ti-6Al-4V is associated with the impingement of slip on boundaries and decohesion of shear bands. To account for these mechanisms, the 3-D crystal viscoplasticity model was further enhanced to address the shear localization and the slip bands (Zhang, 2008). The new crystal plasticity model is described by a two-potential flow rule and takes the dislocation density as the internal variable to determine the hardening and softening behavior of Ti-6Al-4V. This shear-enhanced crystal plasticity model describes slip band formation and propagation using a softening strategy related to the heterogeneity of the microstructure. Several new features such as shear band spacing, evolution of nanoporosity in the shear bands can be considered. The local enriched finite element method is used to model the shear bands in primary α phase. Using this enhanced model, the fatigue performance metrics based on deformation response within the heterogeneous microstructure are more physically based.

Microstructure-based fretting simulations

Fretting contacts, presently considering the partial slip regime, are simulated by a finite element model of a rigid cylinder on an elastic-crystal viscoplastic half-space. The half-space is modeled as duplex Ti-6Al-4V, a polycrystalline alloy consisting of equiaxed primary α grains and secondary lamellar α+β grains. To reduce the computational effort required for the simulations, the crystal viscoplasticity model has only been used in regions near the surface. Both 2-D finite element simulations using a generalized plane strain assumption, which is limited to line contact problems, and fully 3-D finite element simulations have been conducted. Both employ the fully 3-D crystal viscoplasticity model.

2-D finite element simulations – Various realistic 3-D crystallographic textures have been considered (Mayeur, 2004; Mayeur et al., 2008). The deformation fields generated by fretting are quantified in terms of cumulative effective plastic strain distributions and plastic strain maps. The 2-D simulations are carried out for several microstructural realizations with emphasis placed on understanding how texture and tangential force at the interface affect the fatigue life.

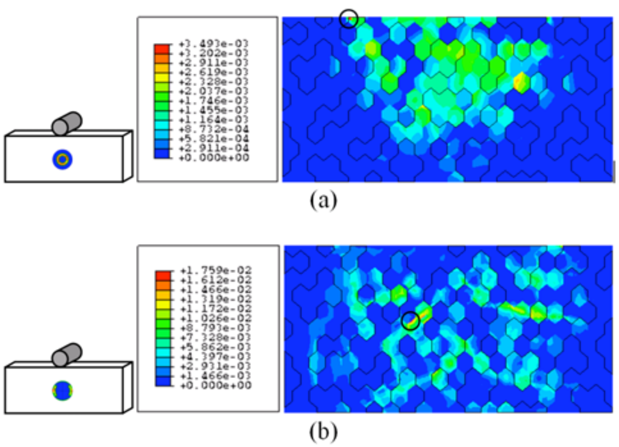

Figure 2. Cumulative effective plastic strain distributions at the end of 3rd cycle, (a) basal texture and (b) transverse texture.

Illustrative results are displayed for the basal and transverse textured materials in Figure 2 (Mayeur et al., 2008). The locations of maximum cumulative effective plastic strain have been highlighted in Figure 2. For all three types of textures considered, ratcheting is observed to be the dominant mode of cyclic plastic deformation. This is in agreement with previous results from crystal plasticity fretting simulations with idealized 2-D textures (Goh et al., 2006a and references therein). The basal textured material exhibits the least amount of plastic ratcheting and correspondingly the most homogeneous distribution of cumulative effective plastic strain. This is direct result of all of the grains for this type of texture being favorably aligned for soft modes of deformation. As a by-product of the relatively homogeneous nature of deformation in the basal textured material, it is able to reach a state of elastic shakedown much earlier than mixed-types of textures. The transverse and basal/transverse textured materials exhibit significantly different behavior. Both of these materials display a highly heterogeneous distribution of cumulative effective plastic strain in the subsurface region (see Figure 2(b)). The plastic strain is partitioned in vein-like "soft" regions of the microstructure in which relatively few favorably oriented grains are surrounded by unfavorably oriented primary α grains and/or the lamellar α+β grains. The confined nature of the plastic strain for the transverse and basal/transverse textured materials leads to continued localized ratcheting as smaller regions of the material are required to accommodate the plastic deformation. The cumulative effective plastic strain is considerably greater in these regions. The results clearly demonstrate the importance of the various sources of microstructural heterogeneity in the surface layers. The main sources of microstructural heterogeneity include grain size, grain size distributions, the volume fraction and distribution of phases, the morphology of the grains and phases, slip system strength anisotropy, and crystallographic texture. Examples of different microstructure realizations are shown in Figure 3.

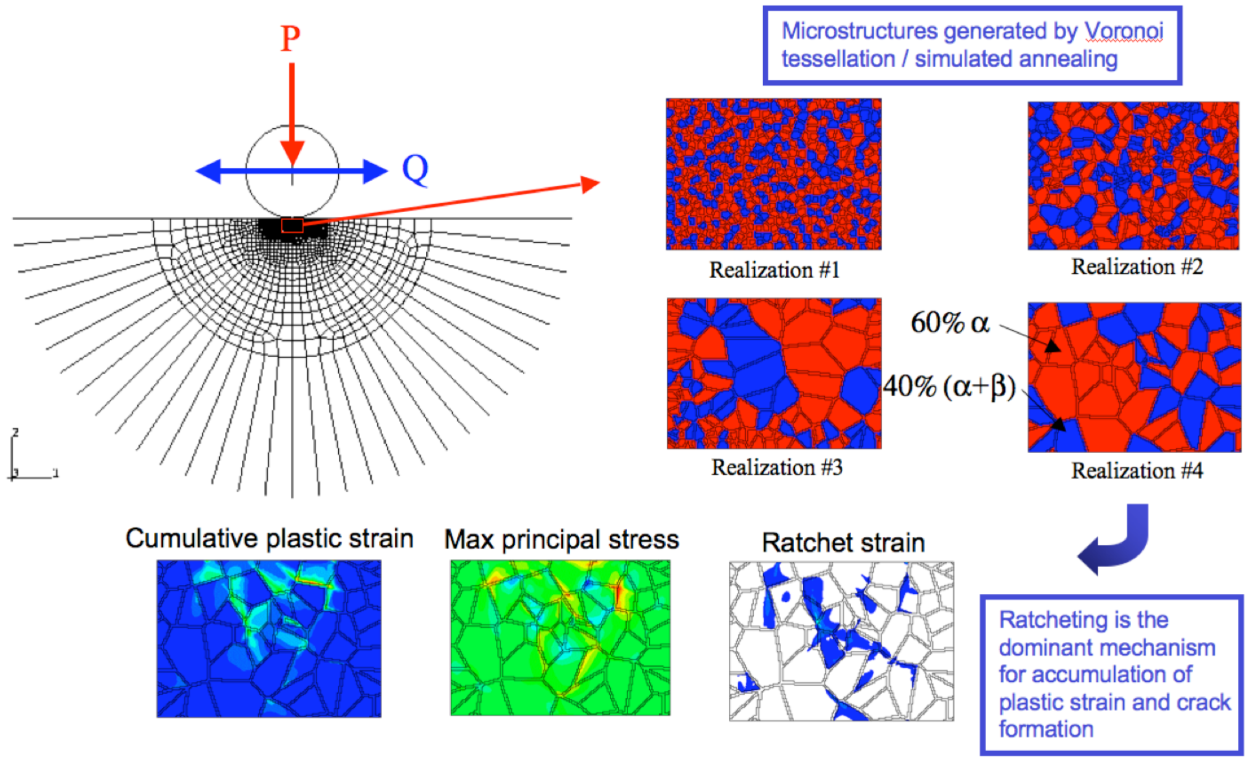

Figure 3. Fretting simulations using crystal plasticity showing examples of different microstructure realizations.

Several fatigue indicator parameters have been considered (Mayeur et al., 2008). Plastic strain-based critical plane parameters are the most relevant when crystal plasticity is used. In addition, both single point and volume-averaged calculations have been considered. The latter tend to temper strong gradients in the near surface stress-strain field and illuminate size effects in fatigue crack formation. The appropriate size of the averaging volume also depends on the microstructure (grain size, phase distribution, contiguity, etc.), the contact loading conditions, and even the coefficient of friction. The parameters are related to the cycles to crack formation according to a modified Coffin-Manson law using data generated in the Air Force High Cycle Fatigue program.

3-D finite element simulations – Fully 3-D finite element simulations were conducted to investigate the applicability of the generalized plane strain assumption that does not represent truly 3-D microstructures and to allow for more complex fretting configurations such as capturing the experimentally observed edge effects along the contact (Zhang, 2008; Zhang et al., 2008a, 2008b).

One example is shown in Figure 4. The contours show localization of the cumulative plastic strain. Some grains significantly yield while the neighboring grains still undergo elastic deformation. The significant contact edge effect can be observed near the surface because in this case the contacting body is shorter in the z-direction than the substrate. At the x-y plane of the half space, the peak cumulative plastic strain is located in the subsurface region, in agreement with the results obtained from the 2-D simulations for a comparable loading case when the tangential force is relatively low.

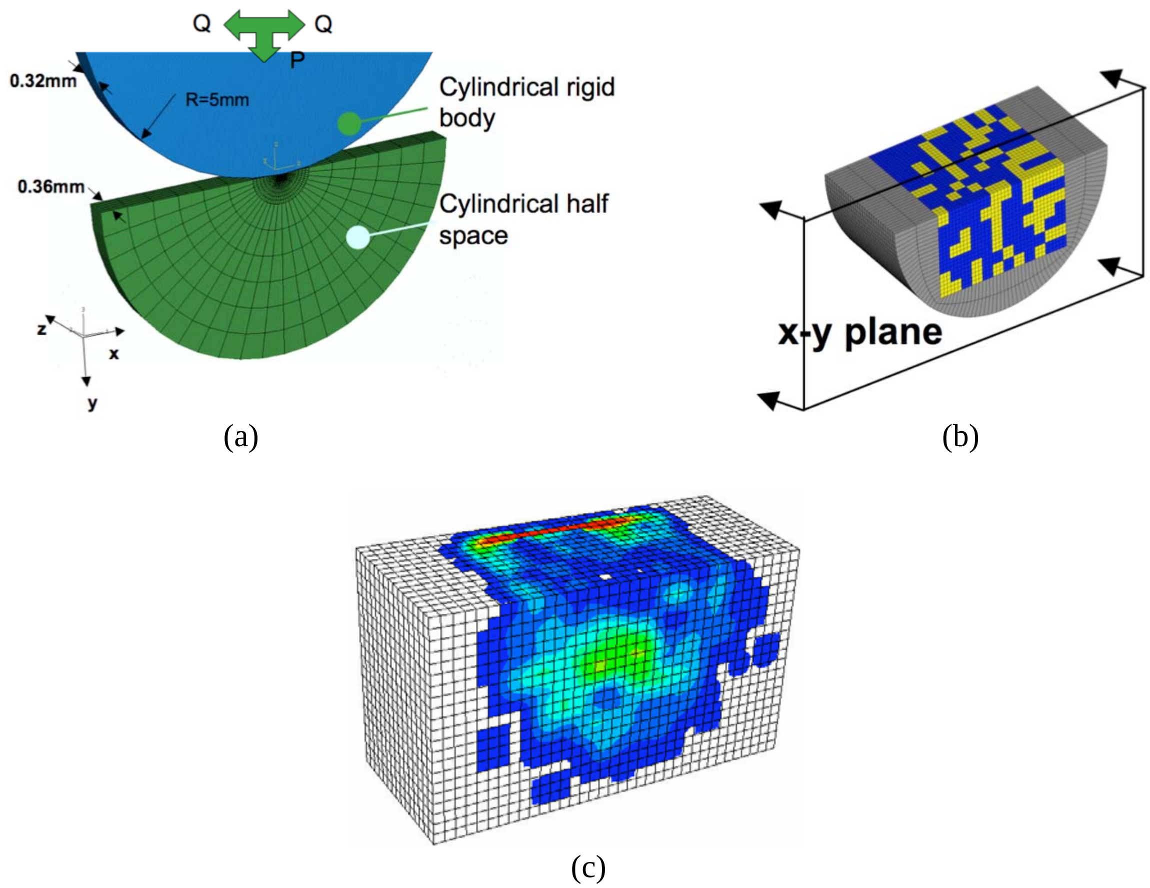

Figure 4. (a) 3-D fretting model. (b) Crystal plasticity region showing the two-phase microstructure. (c) Distribution of cumulative effective plastic strain after three transverse loading cycles for a basal texture case.

This methodology can be used to explore the sensitivity microstructure variations on fretting fatigue performance. In particular, we studied the influence of grain size, grain size distribution, and crystallographic texture on how variations in these affect the drivers for fatigue crack formation using microstructure-based fatigue indicator parameters (Zhang et al., 2008a). Other microstructure attributes could also be considered with this methodology. These include volume fraction of phases, differences in the distribution of primary α and lamellar colony sizes, thicknesses of the α and β lathes, different spatial distributions of microstructural features, and so on. Voronoi tessellation is used to construct the three-dimensional finite element models with different grain size distributions. The results suggest that crystallographic texture has the greatest influence on the plastic deformation and fretting fatigue behavior, while grain size has a mild effect and interestingly the grain size distribution has little influence, likely because the fretting stresses are highly localized. Ratcheting is observed to be the dominant mode of cyclic plastic deformation, which is in consistent with the previous results obtained with 2-D finite element models.

Fretting and shakedown maps

Fretting and plastic strain behavior maps were reevaluated in light of 3-D modeling (Zhang et al., 2008b). Originally, these maps were developed based on idealized 2-D crystal plasticity model of Ti-6Al-4V in our prior AFOSR project. With the more realistic model, the trends are the same, though elastic shakedown is even more difficult to achieve in the less constrained fully 3-D fretting simulations. This suggests that the threshold on fretting crack formation is tied to the size of the fretting process volume since even quite mild fretting conditions exhibit some accumulation of ratchet strain though in highly localized regions of the microstructure. A new fatigue indicator parameter based on the ratchet strain and normal stress on the critical plane, averaged over a domain comparable to the colony size, is suggested. Using this parameter, the driving force for fretting crack formation increases with either increasing normal force or tangential force amplitude. The tangential force amplitude is shown to have the larger influence on crack formation, particularly when the normal force is low.

Experimental characterization of fretting damage

The high temperature fretting machine (DURIP grant F49620-03-1-0260), shown in Figure 5, was used to better understand the role of microstructure in the fretting damage process. This machine has a considerably higher normal force capacity (4500 N) than typical tribometers used in conventional fretting studies, which results in a larger volume of microstructure being distressed by the fretting process facilitating microstructure characterization using pressures relevant to the dovetail attachment between blades and discs in gas turbine engines. For this reason, it has attracted much attention by both military and commercial industries (e.g., General Electric Global Research, Dana Corp., Honeywell Turbo Technologies, Deloro Stellite Group, Federal-Mogul, …).

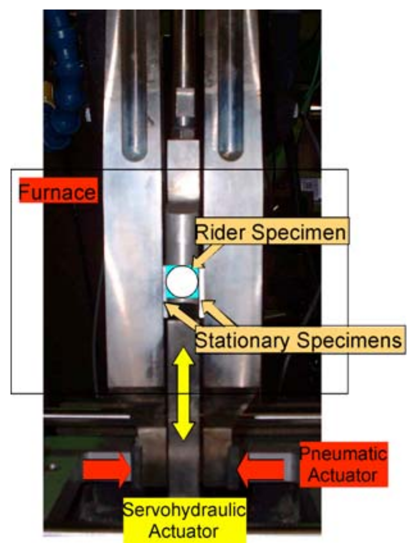

Figure 5. Fretting test machine.

To validate some of the fretting modeling using crystal plasticity, an experimental study of fretting of Ti-6Al-4V on Ti-6Al-4V in point and line contact at room temperature in air was conducted spanning the partial slip, mixed slip, and gross slip regimes of fretting (Huang and Neu, 2008). Cracks are typically observed in the mixed slip regime. The mouths of the cracks are typically wide, indicative of the large plastic ratchet strains in the surface layer, which corroborates predictions using crystal plasticity.

Two methods were used to establish the running condition response of Ti-6Al-4V on Ti-6Al-4V: a conventional multiple specimen approach and an incremental displacement method using a single specimen (Huang and Neu, 2008). It was found that the displacement amplitude corresponding to the transition from partial to gross slip is the same for both methods, and the normal force, at least for values of P/P_y ranging from 1.4 to 3.5, does not significantly affect the coefficient of friction. The running condition and material response at 260°C is essentially the same as the room temperature response (Huang and Neu, 2008). Surface cracks are observed when the displacement amplitude is near the transition between partial and gross slip. Significant fretting wear occurs in the gross slip regime. In our heavy loaded cases, multiple cracks are observed near the edges of contact at 10^4 cycles under mixed fretting conditions. A significant oxide debris layer forms by 10^6 cycles, which is not present at 10^4 cycles. The depth of the oxide debris layer is comparable to the depth of cracks formed at 10^4 cycles, suggesting that crack formation and filling of cracks with oxide debris precedes generation of complete oxide debris layers.

Automated electron backscatter diffraction (EBSD) is used to establish how fretting spatially evolves microtexture and the relationship between crystallographic orientation, grain boundaries and formation of subgrains and cracks in the fretting process volume (Swalla and Neu, 2006). It is a useful tool to quantify evolution of strain-induced microstructural changes due to deformation in the near-surface layers. One notable observation is the appearance of low angle misorientations (<5°) near the fretted surface that tend to increase with increasing slip amplitude (Swalla and Neu, 2006). The development of these intra-grain misorientations in medium to high stacking fault metals is due to the formation of dislocation substructures with accumulated plastic deformation. The relationship between these intra-grain misorientation parameters and plastic strain appear to be linear. We developed a method to establish the correlation using a shear-dominated torsion experiment, which is more relevant to the shear-dominated loading in fretting and sliding contacts. These methods aid in quantitatively interpreting the fretting results and could eventually be used to calibrate material parameters in evolutionary equations in a crystal plasticity model that captures the formation of these dislocation substructure features.

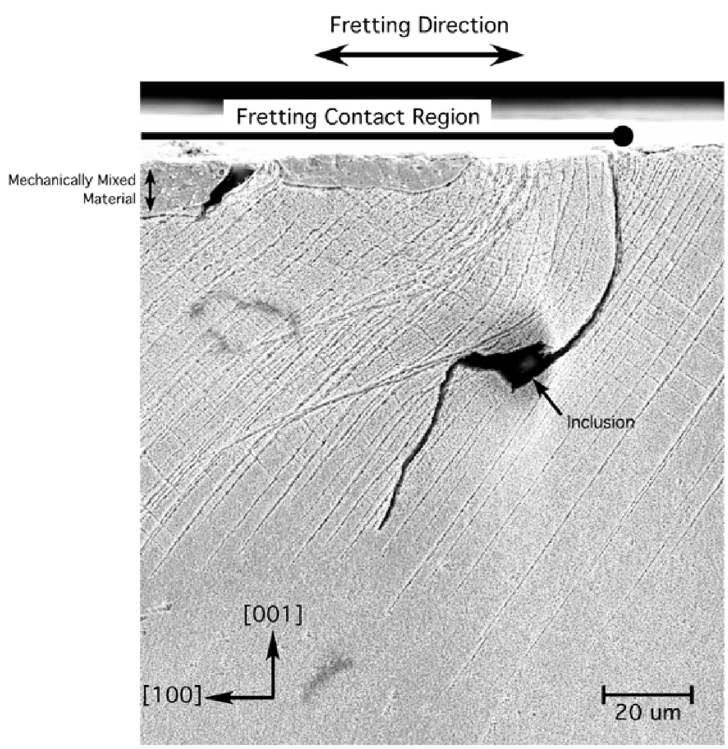

Figure 6. Fretting fatigue crack near edge of contact in a single crystal Ni-base superalloy, etched to show the slip traces.

To establish the role of crystallographic orientation on the fretting damage response, a fretting study on single crystal Ni-base superalloy, PWA 1484, was conducted (Huang et al., 2008). In particular, fretting was conducted on the (001) crystal plane in two directions representing the extreme responses on this plane: the ⟨100⟩ and ⟨110⟩ crystal directions. The response for fretting in the ⟨100⟩ direction is shown in Figure 6. A crystallographic effect on the fretting response was observed at highest normal force ($P > P_y$), while there was no crystallographic effect observed at the lower normal force ($P < P_y$). When the friction depended on crystallographic orientation, the friction on the cubic face in the ⟨110⟩ direction was larger than in the ⟨100⟩ direction. This difference can be explained by the extent of plastic deformation in the surface layer and associated microstructure changes, both of which depend on the coupling between the crystallographic orientation and the cyclic deformation field. Crystal plasticity and relevant lower microstructure length scale models are necessary to predict these observations.

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Zhang, M., Neu, R.W., and McDowell, D.L., "Microstructure-based modeling: application to fretting fatigue," Plasticity 2008, Kailua-Kona (Big Island), HI, January 3-8, 2008, pp. 148-150.

McDowell, D.L., "Scales and Modeling of Metal Fatigue Processes," QuesTek Innovations LLC, Evanston, IL, March 19, 2008.

Neu, R.W., "Microstructure-based Modeling of Fretting Fatigue," ASME Chattahoochee Symposium on Contact Mechanics, Auburn University, Auburn, AL, April 17, 2008.

Neu, R.W., "Microstructure-based Modeling of Fretting Fatigue," Siemens, Orlando, FL, June 3, 2008.

Neu, R.W., Dawkins, J.J., and Zhang, M., "Applications of crystal plasticity in contact mechanics," proc. STLE/ASME International Joint Tribology Conference (IJTC2008), Miami, FL, October 20-22, 2008, Paper Number IJTC2008-71123.

Honors/Awards

Richard W. Neu

American Society of Mechanical Engineers (ASME)
- Orr Best Paper Award, 2006

TAPPI Engineering Conference
- Stowe Best Paper Award, 2006

David L. McDowell

American Society of Mechanical Engineers (ASME)
- Orr Best Paper Award, 2006

Elected Fellow of the Society of Engineering Science (SES), 2007 (at that time, one of 34 Fellows elected since its inception in 1976).

2008 Khan International Medal for outstanding life-long contributions to the field of plasticity

Elected Fellow of ASM International, 2008