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Final Performance Report

LENGTH SCALE CONSIDERATIONS IN THE FORMATION OF ATTACHMENT FATIGUE CRACKS

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Summary

Fretting fatigue is often the root cause of nucleation of high cycle fatigue (HCF) cracks in clamped components. Fretting fatigue damage accumulation occurs within depths of only a few grains at the interface between contacting components. Therefore, more accurate assumptions concerning length scale, damage volume, and material models are needed to establish a more solid physical foundation underlying fretting fatigue life prediction methods. In particular, the influence of crystallographic orientation distribution on the plastic deformation field is significant, as is size of grains or second phases. In this program, 2D and first generation 3D crystal plasticity models are developed for Ti alloys and used to simulate the fretting process. Experimental observations of fretting fatigue crack formation reinforces the results of predictions obtained using computational crystal plasticity models in fretting simulations. New experimental observations are reported regarding the evolution of crystallographic orientation, microhardness, composition, and grain size on duplex Ti-6Al-4V specimens subjected to a range of fretting loading conditions, over a range of crycles.

The importance of crystal plasticity as a simulation tool for fretting fatigue is demonstrated by comparing to conventional simulations of fretting using homogeneous elastic-plastic material models. The fretting simulations in this program have shown for the first time that ratcheting of plastic strain plays a key role in the physics of fretting fatigue crack formation and early growth, corroborated by experimental observations. Fretting and shakedown maps are generated to understand how the various fretting parameters such as normal force and cyclic tangential force amplitude relate to the fretting damage mechanisms. In addition, several simulations have been conducted to examine the role microstructure on fretting, including crystallographic grain orientation distribution (i.e., effect of different initial textures), grain size and shape distributions, and phase distributions.

Fretting experiments conducted on duplex Ti-6Al-4V, Ti-5Al-2.5Sn, and CP Ti shed light on the effects of initial microstucture and how it evolves in the fretting disturbed layer where fretting crack formation typically occurs. This was the first study to use electron backscatter diffraction (EBSD) to detect microstructural changes due to fretting. Important new results include the development of a preferred crystallographic orientation and an increase in low-angle misorientations that depends on fretting displacement amplitude and cycles.

A 3D crystal plasticity model for $\alpha + \beta$ Ti alloys has been developed and implemented as a UMAT subroutine for ABAQUS. The necessity of developing a three-dimensional model capable of representing arbitrary crystallographic textures, the unique crystallography of the constituent phases, anisotropy of elastic stiffness and slip system strengths, and tension-compression asymmetry is essential to capturing the deformation behavior of these materials due to the low symmetry of the hcp crystal structure and the resulting anisotropic properties. Several preliminary simulations investigating the uniaxial response and polycrystalline response with different initial textures have revealed several features of the interplay of the various sources of anisotropy.

Research Objectives

- To improve the understanding of the relationship of microstructure and fretting-related deformation mechanisms through characterization of subsurface deformation and microstructure evolution, as well as damage, generated in fretting experiments in Ti alloys and CP Ti.
- To simulate fretting using finite element methods that incorporate 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.
- To validate the modeling approach by comparing simulations to experiments, and to explore construction of fretting maps that indicate dominant deformation mechanisms, fretting regimes, and links to potential damage mechanisms.

Accomplishments and New Findings

Fretting Simulations: Homogeneous Versus Crystal Plasticity Models

In this work we have shown that 2D polycrystal plasticity simulations of fretting exhibit several significant features that are not manifested by simulations using conventional homogeneous J₂based elastoplastic constitutive models (Goh, 2002). The distribution of cumulative plastic strain using crystal plasticity is considerably more heterogeneous and extends deeper than the distribution predicted by the homogeneous model. Interestingly, the differences between the homogeneous plasticity and crystal plasticity solutions become more pronounced in the high cycle fatigue (HCF) regime as the contact pressure is decreased. The pronounced discrepancy in the HCF regime may be understood largely on the basis that yielding occurs within favorably oriented grains in the microstructure at much lower stress levels in crystal plasticity than for homogeneous plasticity models. As a result, the level of subsurface plasticity predicted by crystal plasticity in such grains is an order of magnitude greater than that predicted using a homogeneous plasticity model. Elastic shakedown limits are predicted to be considerably lower when crystal plasticity is used compared to those predicted using homogeneous plasticity. Moreover, subsurface plasticity becomes a much more serious consideration based on crystal plasticity results. Hence, in the HCF regime, homogeneous (J_2) plasticity models are only slightly more relevant than the purely elastic solution, at least relative to the large differences predicted using crystal plasticity theory.

The most severe location for fretting damage is expected at the boundary between slip and stick, where the largest degree of plastic deformation occurs. It appears to be physically favorable for cracks to initiate near this region. It is interesting to note that the stick/ slip boundary is not a single point; rather, a narrow zone of mixed stick and slip prevails, with small regions of slip appearing within stick regions. It is emphasized that the mixed stick/ slip contact zone can only be predicted using the crystal plasticity algorithm, since gradients in contact force along the contact surface are due to variations of yielding associated with crystallographic orientation of surface grains. It cannot be predicted, for example, using initially isotropic J_2 cyclic plasticity theory and an initially smooth contact surface. The mixed stick/ slip contact zone explains multiple crack nucleation sites observed in experiments. Another implication of this new result is that the plastic deformation predicted by the crystal plasticity model naturally leads to a surface roughness from an initially smooth surface without the need to employ any ad hoc

asperity size and spacing assumptions. This could potentially open the door to new methods of developing models for evolution of the local friction coefficient along the contact.

The Role of Plastic Ratcheting in Fretting Contacts

Crystal plasticity simulations of fretting indicate that ratcheting of plastic strain is an important mechanism in the fretting fatigue process, in contrast to sole influence of a reversed cyclic plasticity damage mechanism, which is predicted by conventional homogeneous plasticity models. The ratcheting arises from the nature of the contact boundary conditions, coupled with the enhanced shear localization largely due to local microstructural constraints (i.e., heterogeneity of orientation of slip), and from the low strain hardening characteristic of the material, as well as the use of a viscoplastic potential in the crystal plasticity case that admits some viscous ratchetting behavior. Experimental observations of fretting crack formation also support a ratcheting mechanism early in the fretting process. This study clearly shows (Figure 1) that ratcheting of plastic strain plays a key role in the physics of fretting fatigue crack formation and early growth that must be explored in more detail to develop engineering models of fretting crack formation.



Figure 1: (a) Location near edge of fretting contact, showing multiple nonpropagating surface cracks as well as widening of the crack mouth, which is evidence of plastic strain ratcheting. Plastic strain maps after completion of three fretting cycles ($\mu = 1.5$, $P/P_{\nu} = 2.0$, and

 $Q_a / P_y = 0.45$) illustrate typical differences between (a) homogeneous (J₂) plasticity and (b) crystal plasticity.

Fretting and Shakedown Maps

Fretting maps shown in Fig. 2 are used to summarize results of parametric studies aimed at determining the role of contact load, P, and tangential force amplitude, Q. Crystal plasticity predicts significantly different regions for ratcheting, shakedown and subsurface versus surface plasticity, especially when $P/P_y > 1.0$, where P_y is the normal (contact) force when first yielding occurs based on von Mises criterion. The elastic shakedown limits both in terms of the tangential force amplitude and normal force are considerably lower when a crystal plasticity model is employed compared to a conventional homogeneous model. Interestingly, increasing the coefficient of friction from 0.75 to 1.5 has only a small effect on these maps, mainly shifting the boundary between elastic shakedown and surface plasticity slightly to the left.



Figure 2: Fretting maps based on (a) J_2 plasticity and (b) crystal plasticity simulations of 2D Hertzian fretting contacts ($\mu = 0.75$).

Microstructure Effects in Fretting of Duplex Ti-6Al-4V

Several first order microstructure effects such as grain orientation angle distributions (i.e., different textures), grain size and shape distributions, as well as phase distributions and contiguous globular α cluster size were investigated with crystal plasticity simulations. The polycrystal plasticity algorithm was modified to represent restricted slip transmission through lamellar $\alpha + \beta$ microstructure. In the 2D model, planar triple slip was employed to represent a strong transverse basal texture, dominated by three prismatic systems as a first approximation.

The distributions of the cumulative effective plastic strain $\overline{\varepsilon}^{p}$ obtained from simulations of a single phase and dual phase alloy are compared in Fig. 3. Black lines shown in Fig. 3(a) represent grain boundaries, while the black lines shown in Fig. 3(b) represent the boundaries between the primary α and the lamellar $\alpha + \beta$ phases. Although the same microstructure and orientation angle distributions are assigned, the distributions of $\overline{\varepsilon}^{p}$ are significantly impacted by contiguous primary α and distributions of $\alpha + \beta$ phase.



Figure 3. Distributions of cumulative effective plastic strain below the fretting contact after completion of three cycles for the case of $\mu = 1.5$, $P/P_v = 1.0$, and $Q_a/P_v = 0.3$.

Microstructural Characterization of Fretting Damage

Fretting experiments were conducted on $\alpha+\beta$ Ti-6Al-4V, α Ti-5Al-2.5Sn, and CP Ti to understand the effects of fretting conditions on fretting deformation and damage processes, especially focusing on the effect of initial microstructure and its evolution during the fretting process (Swalla, 2003). Significant plastic deformation occurs within a region very near the fretting contact. This deformation is visually observed in the form of flow patterns, changes in grain size and shape, and rotation of markers. At the edge of the fretting contact, several small cracks form of length ranging from 10 µm to 50 µm. There appears to be a critical threshold of slip amplitude in which oxygen diffusion and grain reorientation very near the fretted surface, among other factors, combine to make conditions more favorable for crack formation. This was the first study to use electron backscatter diffraction (EBSD) to detect microstructural changes occurring due to fretting. Important new results include the development of a preferred an increase in low-angle misorientations, crystallographic orientation, and grain distortion/refinement. As shown in Figure 4, a strong microtexture develops within approximately 30 μ m of the fretted surface when the relative slip amplitude is greater than ±15 µm and number of cycles is equal to or greater than 10⁴. In fretting tests where $\delta \ge \pm 60$ µm, a basal or nearly basal texture forms (i.e., [0001] direction and ND coincide) at a location near the center of contact.

The fretting disturbed layer in Ti-6Al-4V is 5% to 20% softer than the bulk virgin material based on nanoindentation studies (Figure 5). This latter result may be attributed to the formation of basal texture noted earlier (keeping in mind that indentation is being done in the TD), the depletion of Al due to the oxidizing process, and/or cycle-dependent softening. Even in the virgin region, the hardness varied and the crystal plasticity simulations of fretting indicate that the heterogeneity in these properties leads to a concentration of localized accumulated deformation, significant as a precursor to formation of cracks. The higher measured hardness values tended to occur near grain boundaries and/or in $\alpha+\beta$ lamellar colonies.



Figure 4: Pole figures for (a) as-received cross section, (b) area away from fretted surface in Test 1 ($\delta = \pm 60 \mu m$, N=10⁵ cycles), and (c) area within about 30 μm of fretted surface in same test.



Figure 5: Nanoindentation study near interface of fretting contact showing the reduction of hardness on average in the near surface layer with some areas of higher hardness highlighted.

Misorientation Angle Distribution

In the fretting disturbed region below an oxidized layer, there is a sharp increase in low-angle misorientations ($< 5^{\circ}$) that indicates the formation of subgrains, as shown in Figure 6. The distribution of low-angle misorientations in deformed metals has been linked to the evolution of plastic strain. It may be possible to use the misorientation distribution obtained by EBSD to correlate plastic strain due to fretting and to explicitly link experimental and computational analysis results. This measure has the potential to improve damage assessment estimates in fretted components.



Figure 6: Change in misorientation angle distribution with fretting.

Development of a 3D Crystal Plasticity Model for HCP Materials

A three-dimensional crystal plasticity model for the dual-phase (α + β) Ti-Al alloy, Ti-6Al-4V with duplex microstructure was developed and is currently being implemented (Mayeur, 2004) as a UMAT subroutine for ABAQUS (2003). The necessity of developing a three-dimensional model capable of representing arbitrary crystallographic textures, the unique crystallography of the constituent phases, elastic anisotropy, anisotropy of slip system strengths, and tension-compression asymmetry due to non-planar dislocation core structures in primary α and/or directionality of ease of slip transmission through the bcc β phase in α + β is essential to capturing the deformation behavior of these materials due to the low symmetry of the hcp crystal structure and the resulting anisotropic properties. They are also needed to assess the utility and limitations of the idealizations made in 2D modeling. Most of the work during the period of performance has centered on model development and parameter sensitivity studies under uniaxial loading conditions to provide intuition into the fundamental aspects of deformation and

the interaction of the various sources of anisotropy. Ultimately, the goal of this research is to apply the model to the problem of predicting the location and mechanisms of crack initiation during attachment fatigue with three-dimensional textures and microstructures.

In the 3D model the primary α -phase has 24 active slip systems: 3 basal, 6 prismatic, 6 firstorder 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 necessary to fulfill requirements for representing arbitrary inelastic deformation rates. Mobility of screw dislocations controls slip in this alloy at room temperature, and slip has a coarse, somewhat planar nature. It has also been observed that single crystal titanium aligned for prismatic slip exhibits non-Schmid behavior (Naka et al., 1988) and it has been speculated that the prismatic dislocation core is non-planar, depending on interstitial oxygen level. In accordance with these observations, the dislocation core model of Naka et al. (1988) has been employed, assuming dislocation dissociation from the prismatic plane into two first-order pyramidal planes. Such a configuration is sessile and requires recombination via constriction stress in the prismatic plane before slip can continue.

The precise nature of slip in the lamellar $(\alpha+\beta)$ phase is not as well understood as that within the primary α phase. The lamellae are not explicitly represented in this model as this would be prohibitive in the finite element meshing of a polycrystal simulation. Instead these regions are represented implicitly by including both hcp and bcc slip systems, aligned according to a Burgers orientation relation, in an equivalent pseudo-hcp model. These $(\alpha+\beta)$ grains also have 24 slip systems: 3 basal, 6 prismatic, 6 first-order pyramidal <a>, and 12 (110)[111] bcc slip systems, with special assumptions for slip transmission through α/β interfaces. It is believed that these lamellar regions, and more specifically the α/β interfaces, are responsible for improved fatigue properties. The actual source of the strengthening mechanism is still a subject of debate in the literature. Some researchers have attempted to link the strength of the lamellar colonies via a Hall-Petch type relation (Brockman, 2003; Dimiduk et al. 2001) (most notably for γ -TiAl alloys) and others have argued that the interfaces act as significant obstacles to slip transmission (Savage et al., 2001; Ambard, 2001) for unfavorably aligned slip systems. A mixture of both philosophies is employed in this model.

The flow rule and evolution equations for the α^{th} slip system are given by

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_{o} \left\langle \frac{\left| \tau^{\alpha} - \chi^{\alpha} \right| - \kappa^{\alpha}}{D^{\alpha}} \right\rangle^{m} \operatorname{sgn} \left(\tau^{\alpha} - \chi^{\alpha} \right)$$
(1)

$$\kappa^{\alpha} = \begin{cases} \kappa_{o}^{\alpha} + A\left(\tau^{\{10\bar{1}1\}} - \tau^{\{10\bar{1}\bar{1}\}}\right), \text{ for prismatic systems} \\ \kappa_{o}^{\alpha} & \text{otherwise} \end{cases}$$
(2)

$$\kappa_{\rm o}^{\alpha} = k_{\rm y} / \sqrt{d^{\alpha}} \tag{3}$$

$$\chi^{\alpha}(0) = 0, \qquad \dot{\chi}^{\alpha} = h\dot{\gamma}^{\alpha} - h_{D}\chi^{\alpha} \left\| \dot{\gamma}^{\alpha} \right\|, \quad \dot{\kappa}^{\alpha} = 0, \qquad \dot{D}^{\alpha} = 0$$
(4)

Here, $\dot{\gamma}^{\alpha}$ is the slip system shearing rate, $\dot{\gamma}_{o}$ is a reference shearing rate, τ^{α} is the resolved shear stress, χ^{α} is the slip system back stress (very small compared to threshold stress), κ^{α} is the slip system threshold stress, d^{α} is a measure of length scale associated with mean free path for slip (e.g. lamellae width in the $(\alpha+\beta)$ phase in the slip direction, grain size in primary α and so on), and D^{α} is the slip system drag stress. As noted in the equations above, the threshold stress for prismatic systems in primary α is modified to include the non-Schmid dependence, as the shearing rate on these slip systems depends on the resolved shear stress of first-order pyramidal planes as well. For non-prismatic systems and prismatic systems in the $(\alpha+\beta)$ grains the threshold stress is a constant determined by the grain size and/or lamellae thickness (i.e., A = 0). The drag stress is taken as a constant for each family of slip systems, but takes on different values depending on the relative ease of glide on the particular slip systems. The formulation in Eqs. (1)-(4) is unique in its assignment of Hall-Petch scale effects via the threshold stress, with the drag stress playing the role of rank ordering overall slip system resistances in accordance with experimental data for polycrystals. There are potential issues in direct measurement of slip system characteristics (strength, hardening rates) using small scale single crystal or single colony samples machined, for example, using focused ion beam methods to deliver information of quantitative quality to support identification of parameters in slip system level relations in view of in situ interactions of low symmetry phases and interfaces, so the approach taken here seems quite reasonable.

Preliminary simulations investigating the uniaxial response of the model have revealed several interesting features of the interplay of the various sources of anisotropy. In these simulations, the deformation behavior of four characteristic textures has been evaluated: random, basal, transverse, and basal/transverse. A series of parametric studies 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 has revealed that the activation of slip systems other than prismatic dominate the material yield and work hardening behavior. In these simulations, the CRSS for the prismatic systems is held constant, while the CRSS for the other families of slip systems is prescribed as a multiple of the prismatic CRSS. For example, the yield strength increases by ~10% with a 50% relative increase in the basal CRSS. Another simulation result is that no significant macroscopic tension/compression asymmetry exists for polycrystals, in contrast to experimental observations. Due to inclusion of non-Schmid terms, single crystal simulations of a crystal optimally aligned for prismatic glide exhibit 15% difference in the yield strengths in tension and compression. The fact that only a 3-5% difference exists in the yield strengths in tension and compression in polycrystal simulations indicates that the prismatic slip systems do not dominate this behavior. It has been determined that the only significant effect of the non-Schmid terms on the polycrystalline material behavior is to facilitate strain localization in regions where prismatic slip systems are favorably aligned. Another interesting aspect of the deformation behavior based on these simulations is that the macroscopic flow stress levels at higher strains (>3%) are dictated by the CRSS of the first-order pyramidal <c+a> systems. This result is consistent with experimentally observations in these materials at higher strain levels, as the <c+a> slip systems are often associated with sustaining compatibility at grain boundaries as deformation continues

and lattice rotation begins to occur. The yield strength is essentially unaffected by increases in the CRSS for these systems.

Polycrystal simulations have also been carried out employing the dual-phase representation of the microstructure with basal, transverse, and basal/transverse textures to determine the dependence of the textured material behavior on loading direction. Although these simulations were not fit to any specific set of experimental data, they were able to accurately reproduce the dependence of the elastic modulus and macroscopic yield strength (Peters et al., 1984) on These simulations also show the desired result that the majority of the plastic texture. deformation is contained within the contiguous regions of the primary α phase, also consistent with experimental observations. At this point we are proceeding with fretting simulations for 3D textures. The aim of this work is determine how the subsurface deformation field is affected by the dual-phase representation of the microstructure imbued with realistic three-dimensional textures. Quantification of the deformation field will be achieved by examining the cumulative plastic strain distributions, constructing plastic strain maps, and evaluating plastic strain-based multiaxial fatigue parameters. The model has been calibrated with cyclic Ti-6Al-4V data from Kurath (1999) and Wisniewski et al. (2004) (data were taken from Swalla (2003) as well) for a randomly textured polycrystalline sample of duplex microstructure. Once the model was calibrated, simulations were performed using the 3D model generalized plane strain for basal, transverse, and basal/transverse textures, as shown in Figure 7. Visual inspection of the results for preliminary 3D fretting simulations, shown in Figure 8, support the conclusion of Goh (2002) that plastic ratcheting is a dominant mechanism in attachment fatigue that may lead to crack initiation via a ductility exhaustion mechanism.

The experimental characterization of fretting damage is used to further understand the process of fretting and to validate and interpret the predictions of crystal plasticity in simulating fretting. A new DURIP-funded high temperature fretting machine (grant F49620-03-1-0260) expands our range of normal and tangential loading conditions and allows the study of temperature and environmental effects, as we look to the next phase of the fretting fatigue program. This is important since even a moderate increase of temperature to 200°C results in a 25% decrease in the cyclic yield strength in Ti-6Al-4V (Wisniewski et al., 2004). Orientation imaging microscopy (OIM) 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, 2003). A damage measure using the misorientation angle distribution obtained by OIM based on EBSD is also being established. Nanoindentation is used to assess the spatial changes in mechanical properties. These experimental results will both help refine the material parameters and evolution relations in our 3D crystal plasticity models as well as validate the results of the fretting simulations.



Figure 7: Common crystallographic textures for Ti-6Al-4V plate.



Figure 8: Subsurface 3D fretting deformation maps for a selected fretting loading condition and several 3D textures.

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Swalla, D.R. and Neu, R.W., "Application of orientation imaging microscopy in assessing fretting damage," proc. 9th National Turbine Engine High Cycle Fatigue (HCF'04), Pinehurst, NC, 16-19 March, 2004.

Neu, R.W., McDowell, D.L., Mayeur, J.R., Goh, C.-H., and Swalla, D.R., "Fretting Fatigue of Ti-6A1-4V: A Micromechanical Approach," 2nd U.S.-Korea Workshop on Advances in Metallic Structural Materials, May 11-13, 2004.

Swalla, D.R. and Neu, R.W., "Fretting damage assessment of titanium alloys using orientation imaging microscopy," 4th International Symposium on Fretting Fatigue, Lyon, France, 26-28 May 2004.

Neu, R.W., "Fretting Fatigue: Characterization, Life Prediction, and Palliatives," Lockheed-Martin, Marietta, GA, June 15, 2004. (taped for broadcast to other Lockheed-Martin locations)

Neu, R.W. and McDowell, D.L., "Integrating Microstructure in Life Prediction," AFOSR Workshop on Damage Prognosis of Metallic Materials, Washington, DC, 28-30 June 2004.

McDowell, D.L., Neu, R.W., Mayeur, J.R. and Zhang, M., "Microstructure and 3-D Effects in Fretting Fatigue of Ti Alloys," AFOSR review of Metallic Materials Program, Wintergreen, VA, Aug. 16-18, 2004.

Honors/Awards

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David L. McDowell

American Society for Testing and Materials

- Annual Fatigue Lecture, 2002

- Outstanding Service Award, 2001

Georgia Institute of Technology

- Outstanding Interdisciplinary Activities Award, 2001

Jack M. Zeigler Woodruff School Outstanding Educator Award, 2004

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