Linking Computational Multiscale Failure Analyses to Advanced Diffraction Measurements

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Joint Workshop on Large-scale Computer Simulation
by Joint Institute for Computational sciences (JICS) & German Research School (GRS)

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Mechanics is Unique across Scales

Atomistics of asperity indentation
Defects nucleation from steps
Computer design of toughness
Discrete dislocation simulations of friction and wear
FEM with classic plasticity

1) Develop computational methods to simulate mechanical behavior of materials across length scales
2) Solve fundamental problems that elucidate the role of atomic-scale and mesoscale phenomena in deformation and failure of materials
3) Conduct numerical simulations that aid the understanding and the development of experiments, and validate those computational models
Neutron Strain Measurements of Fatigue Crack

- Because of the deep penetration capability of neutron beams, neutron diffraction allows bulk measurements with a typical spatial resolution in the order of millimeters.
- Intergranular (type II) and intragranular (type III) strains from diffraction experiments of a Ni-based superalloy.
- Fatigue simulation + lattice strain evolution.

A Multiscale View of the Crack Tip Plasticity

• We cannot really model all the phenomena near the fatigue crack tip.
• So under what circumstances can we separate the scales, or not?

Outline

Objectives

• A full field comparison between neutron diffraction measurements and finite element simulations will allow us to quantify the plastic deformation behavior near a fatigue crack tip

This work

1) The crystal plasticity model is used to predict lattice strain evolution in uniformly stressed polycrystals
   ❖ Why stress history and stress multiaxiality affects lattice/intergranular strains?

2) An irreversible, hysteretic cohesive interface model is developed to simulate the continuum strain evolution near a fatigue crack tip
   ❖ Provide stress history to crystal plasticity simulations

3) Experimental comparisons – lattice strain distribution near a fatigue crack tip
Crystal Plasticity and Lattice Strain

Using slip-based crystal plasticity, we can simulate lattice strain evolution in Ni-based superalloy (cubic grains, random orientations).

Finite Deformation and Crystal Plasticity

- Multiplicative decomposition

\[ F = F^e F^p \]
\[ F_{ij} = \frac{\partial x_i}{\partial X_j} = F^e_{ik} F^p_{kj} \]

- Velocity gradient

\[ \dot{F}^p F^{p-1} = \sum_{\alpha} \dot{\gamma}^{(\alpha)} s^{(\alpha)} \otimes m^{(\alpha)} \]

- Elasticity

\[ T = \mathcal{J} F^{e-1} \sigma F^{e-T} \]
\[ F^e = \frac{1}{2} \left( F^{eT} F^e - I \right) \]

- Flow rule

\[ \dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left( \frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m} \]

\( \tau^{\alpha} \) is the resolved shear stress of \( \alpha \) slip system

\( g^{\alpha} \) is shear strength of \( \alpha \) slip system

- Hardening law

\[ \dot{h}_{\alpha\beta} = \sum_{\beta} h_{\alpha\beta} |\dot{\gamma}^{\beta}| \]

\[ h(\gamma) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right) \]

\[ h_{\alpha\beta} = h(\gamma) \left[ q + (1 - q) \delta_{\alpha\beta} \right] \]

Peirce, Asaro, Needleman, Acta Met. 1982
Grain-Orientation-Dependent Lattice Strain

- Lattice strains depend on the angle between loading direction and diffraction vector (Wang et al., Nat. Mater. 2003)
- Each angle selects different sets of hkl grains

<table>
<thead>
<tr>
<th>FCC Steel</th>
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<tbody>
<tr>
<td>$c_{11}$ (GPa)</td>
<td>$c_{12}$ (GPa)</td>
<td>$c_{44}$ (GPa)</td>
<td>m</td>
<td>$h_{ij}$ (MPa)</td>
<td>$\tau_{\theta}$ (MPa)</td>
<td>$\tau_{\phi}$ (MPa)</td>
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<tr>
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<td>137.7</td>
<td>126.2</td>
<td>50</td>
<td>205</td>
<td>87</td>
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</tbody>
</table>
Grain-Orientation-Dependent Lattice Strain

- Lattice strains can be understood by Taylor model
- Load partitioning among “hard” and “soft” grains

Zheng et al., in preparation (2012)
A Multiscale View of the Crack Tip Plasticity

- Using computer simulations and neutron strain measurements, we aim to quantify the dependence of surrounding plasticity and fatigue growth behavior on material properties, load pattern, microstructure, etc.
- A numerical tractable formulation is by the decoupling of scales = continuum plasticity simulations of fatigue behavior + crystal plasticity simulations of microstructure and lattice strains.

Hysteretic, Irreversible Cohesive Zone Model

- Cohesive interface model prescribes a set of traction-separation constitutive law for weak interfaces
- Implemented in ABAQUS User-defined EElement (UEL) subroutine

\[ \int \sigma_{ij} \delta e_{ij} dV + \int T_{\alpha} \delta \Delta_{\alpha} dA = \int t^* \delta u dA \]

- An irreversible, hysteretic formulation will introduce a damage mechanism which allows the formation of a fatigue crack

\[ \dot{T}_n = \begin{cases} K^- \dot{\Delta}_n, & \dot{\Delta}_n < 0 \\ K^+ \dot{\Delta}_n, & \dot{\Delta}_n > 0 \end{cases} \]

unloading stiffness \[ K^- = \frac{T_n^{\text{unload}}}{\Delta_n^{\text{unload}}} \]

reloading stiffness \[ \dot{K}^+ = \begin{cases} -K^+ \dot{\Delta}_n / \delta_f, & \dot{\Delta}_n > 0 \\ (K^+ - K^-) \dot{\Delta}_n / \delta_a, & \dot{\Delta}_n < 0 \end{cases} \]

Nguyen et al., Int. J. Fract. 110, 351-369 (2001)
Fatigue Crack Growth and Overload Effects

- The phenomenological cohesive interface model can faithfully reproduce a steady fatigue crack if
  - A plastic wake should emerge and be larger than the plastic zone size
  - Crack increment is much smaller than the plastic zone and crack bridging zone
  - Crack bridging zone is smaller than the plastic zone
- Although a smooth crack growth is predicted, $da/dN$ is far different from experiments
- Preliminary studies on overload effects show crack growth retardation

Example #1: Mises stress for $\delta_f=0.004\text{mm}$

<table>
<thead>
<tr>
<th>$\sigma_{\text{max}}$ (MPa)</th>
<th>$\delta_n$ (μm)</th>
<th>$\delta_a/\delta_n$</th>
<th>$\delta_f/\delta_n$</th>
<th>E (GPa)</th>
<th>$\nu$</th>
<th>$\sigma_Y$ (MPa)</th>
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<td>1</td>
<td>0.4</td>
<td>4</td>
<td>210</td>
<td>0.3</td>
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</table>
Experimental Comparisons – 316 Stainless Steel

- Compressive strain field (averaged over 1mm volume) appears in the plastic wake
- Simulations show a smaller shift of strain distribution than experiments, probably due to the boundary effects in experiments

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<th>(\sigma_{\text{max}}) (MPa)</th>
<th>(\delta_n) ((\mu)m)</th>
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<td>210</td>
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<td>288</td>
</tr>
</tbody>
</table>

Experimental Comparisons – 316 Stainless Steel (cont’d)

Y.N. Sun, PhD thesis, University of Tennessee (2007)
Stress History

- In order to obtain $\epsilon_{hkl}$ distribution, we need to use stress history as inputs for a polycrystal plastic simulation.
Experimental Comparisons – HASTELLOY® C-2000® Alloy

- A representative result is shown for the HASTELLOY C-2000 alloy (58wt.%Ni-23wt.%Cr-16wt.%Mo, single-phase FCC, E=207GPa, Y=393MPa, grain size=90 ± 20 μm)
- The trend of lattice strain <100> & <111> versus the distance from the crack tip curves agrees well with the experiment. There is a cross point near the crack tip, ahead of which $\varepsilon_{100}>\varepsilon_{111}$

#1: $\sigma_{max} = 980\text{MPa}, \delta_c = 0.9\,\mu\text{m}, \delta_f = 22.5\,\mu\text{m}, \delta_s = 0.09\,\mu\text{m}$

#2: $\sigma_{max} = 1,225\text{MPa}, \delta_c = 0.72\,\mu\text{m}, \delta_f = 18.0\,\mu\text{m}, \delta_s = 0.072\,\mu\text{m}$
Role of Stress Multiaxiality

- The evolution of stress multiaxiality along the crack path dictates the lattice strain distributions.

Discrepancies due to “Clean” vs “Messy” Process Zones

- Our simulations intentionally chose small cohesive zones → so that surrounding plasticity is faithfully modeled
- Actual “messy” fracture process zone is due to grain boundary damage, voids, etc.
Materials for Energy Applications at Extremes


Alloy 617 considered for intermediate heat exchanger at 900-950°C for Next Generation Nuclear Plant (NGNP) applications. Decarburized layer, surface crack, and voids formed in purified argon test at 0.3% strain range and 60s tensile hold time (Totemeier and Tian, Mater. Sci. Eng. A, 81, 468-470, 2007).

Challenges: Basic Research Needs for Materials under Extreme Environment


by DOE Basic Energy Sciences Advisory Committee (2007)


A multiscale view of the creep-fracture process. The unit event at the smallest scale is an explicit model of cavitation at grain boundaries.
Creep-Resistant, Ferritic Alloys with NiAl Precipitates

1. Volume-averaged phase strain

\[ \varepsilon_{\text{avg\_phase}} = \frac{a - a_0}{a_0} \]

Rietveld whole-pattern fitting

2. hkl plane specific strain – intergranular

\[ \varepsilon_{\text{hkl}} = \frac{d_{\text{hkl}} - d_{\text{hkl}}^0}{d_{\text{hkl}}^0} \]

Single peak fitting of overlapping composite peak

3. Local phase strain - intragranular

\[ \varepsilon_{\text{local\_}\beta} = \frac{d_{\beta} - d_{\beta,0}^{\beta}}{d_{\beta}^{\beta,0}} \]

Separation of overlapping fundamental reflections

S.Y. Huang, PhD thesis, University of Tennessee (2011)
Loading Partitioning: Intergranular & Inter-phase

1000 cubic grains, random texture
3 x 3 x 3 grid, Vol.% = 18.5%

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<th>$c_{11}$ (GPa)</th>
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<td>precip.</td>
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<td>106</td>
<td>10</td>
<td>--</td>
<td>&gt;500</td>
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</tr>
</tbody>
</table>

- Inter-phase and inter-granular load transfers are coupled
- A dramatic load transfer from matrix to precipitates at 773K after yielding of most similarly oriented hkl grain families

Huang, Gao, et al., in prep. (2012)
Summary

The good:

• The primary challenge in the fatigue study is an in situ, nondestructive measurement on the microstructural length scale, which permits us linking the stress analyses (from a top-down point of view) and the failure mechanisms on inter- and intra-granular scales (from a bottom-up point of view).
   Full field comparison of lattice strains for a fatigue crack tip in Ni-based superalloy
   Inter-granular and inter-phase load transfer in ferritic superalloy

• As opposed to neutron diffraction, the synchrotron x-ray diffraction is more ideal to study intergranular damage and intragranular deformation heterogeneity (i.e., short cracks, crack initiation, etc.)

The bad:

• Separation of length scales must be valid → we really cannot do a full field simulation on the grain level
• Not suitable for short cracks because of complicated fatigue mechanisms