Archetype-Blending Multiscale Continuum Method

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Outline

• Background and Motivation
• Archetype-Blending Continuum (ABC) Theory
• Computational Fatigue
• ABC microplasticity simulation
• ABC fatigue simulations
• Conclusions
Motivation and Background

Microstructure

Macrostructure

1 Porter, Easterling, 2004
Fatigue in Biomedical Stents

Notch Effects

Un-notched

Notched

\[ \text{Stress, } S \] vs. \[ \text{Log Life, } N \]

\[ \frac{S}{K_t} \]

\[ \div K_f \] Fatigue Notch Factor

\[ \div K_t \]
Neuber’s Equation

Notched

\[
\frac{K_f}{K_t} = \frac{1 + \frac{1}{K_t} \sqrt{A/\rho}}{1 + \sqrt{A/\rho}}
\]

Material dependent Non-linear

Non-linear material dependent behavior indicates microstructural dependence

Schijve, Fatigue of Structures and Materials, 2001
Fatemi-Socie in 1988 proposed a fatigue indicating parameter (FIP) to account for discrepancies in $\varepsilon$-$N$ curves due to loading condition.

\[ \gamma_f(2N)^c = \left(1 + K' \frac{\sigma_{max}^n}{\sigma_y} \right) \frac{\Delta\gamma_{max}^p}{2} \]

- **Empirical Constant**
- **Material Parameter**
- **From FEM/Experiment**

Fatemi and Socie Fatigue & Fracture of Engineering Materials & Structures, 1988
Fatigue Regimes

• Total fatigue life is broken into three regimes\(^1\)
  \[ N_{Total} = N_{Inc.} + N_{MSC} + N_{LC} \]

• Incubation (\(N_{Inc.}\)): nucleation and growth of crack beyond influence of microstructural notch\(^1\)
  – Characterized by microscale plastic strain and nonlocal damage parameters

• Microstructurally Small Cracks (\(N_{MSC}\)) : growth of crack from incubation size \(a_i\), such that \(a_i < a < kG_S\), where \(k\) is (1-3) and \(G_S\) the lengthscale of a grain or other prominent microstructural features\(^1\)
  – Characterized by elasto-plastic fracture mechanics

• Long Cracks (\(N_{LC}\)) : macroscopic crack growth\(^1\)
  – Characterized by linear elastic fracture mechanics

This slide was not originally presented on 3/4/2014

1 Horstemeyer, ICME for Metals, 2012
Treatment of Fatigue Regimes

• Total fatigue life is broken into three regimes
\[ N_{Total} = N_{Inc.} + N_{MSC} + N_{LC} \]

• The following work will address only \( N_{Inc.} \) as it accounts for a large % of fatigue life for many alloys

• The ABC theory will be able to model the \( N_{MSC} \) and \( N_{LC} \) regimes by:
  – Studying several (5-10) initial cycles and determining \( N_{Inc.} \) from a FIP
  – Using this as an initial state for explicit modeling of \( N_{MSC} \) and \( N_{LC} \)
  – \( N_{MSC} \) region could be considered 1 element (\( k_{GS} = 1 \) element) and growth modeled with methods such as XFEM
  – Once crack grows beyond 1 element \( N_{LC} \) can be modeled based on basic damage models, strain gradients in ABC will aide in regularization (reducing mesh sensitivity) and localization

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This slide was not originally presented on 3/4/2014
Direct Numerical Simulation of FIP

Zhang's Mesh

Fatigue Theory Summary

• Linear Elastic Theory
  – Overly conservative
  – No material information
  – No microscale information

• Neuber’s Theory
  – Require extra material tests
  – Only works for simple notches
  – No microscale information

• Fatemi-Soci (FIP) Theory
  – No macroscale notch information
Archetype-Blending Continuum (ABC) Theory

- Combines generalized continuum mechanics and constitutive modeling
- Degrees of freedom represent partitions of microstructure
- Each degree of freedom is similar to assembly of Eshelby problems in micromechanics but strain are determined by solving equations of motions
- Virtual Power

\[ \delta P_{int} = \int_{\Omega} \left( \sigma : \delta \hat{L} + \sigma \sigma : \delta \hat{L} \nabla + s^n : \delta \hat{L}^{n} + ss^n : \delta \hat{L}^{n} \nabla \right) d\Omega \]


03/24/2014
Steel Research Group 30th Annual Meeting
Non-linear reduction in S-N curve is:
- Material dependent
- A function on macroscale strain gradients
- A function of microscale strain gradients

\[ \delta P_{\text{int}} = \int_{\Omega} \left( \sigma : \delta \hat{L} + \sigma \sigma : \delta \hat{L} \nabla + s^n : \delta \Lambda^n + ss^n : \delta \Lambda^n \nabla \right) d\Omega \]

Models

10% volume fraction

300MPa

1% volume fraction

Ramped Velocity: 7571 m/s

$\gamma$
Implicit Microstructure

Matrix: Young’s Modulus: 200 GPa
Yield Strength : 250 MPa

Interphase: Young’s Modulus: 200 GPa
Yield Strength : 250 MPa

Inclusion: Young’s Modulus: 2000 GPa
Linear Elastic

Degree-of-Freedom 1 \( \varepsilon^1 \) Matrix
Degree-of-Freedom 2 \( \varepsilon^2 \) Interphase

\( \mathcal{E} (\varepsilon^2) \) Inclusion

\( \mathcal{E} = \) mapping of strain using Eshelby’s solution
Microplasticity

matrix

interphase

inclusion

300MPa

$\varepsilon_{\text{eq}}$ vs. $X$

$\varepsilon_{\text{eq}} = 6 \times 10^{-4}$
Response of Notched Sample

Linear Elastic Macro Stress

Equivalent Plastic Interphase Strain

Stress w/o notch is 300 MPa,

\[ K_t \approx 2 \]

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<th>15</th>
<th>149</th>
<th>283</th>
<th>417</th>
<th>596</th>
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0 0.4 0.8 1.4 1.8 x10^{-3}
Notched Sample Fatigue Prediction

![Graph showing fatigue life prediction models](image)

- **ABC, FIP (un-notched)**
- **Linear-Elastic**
- **Neuber**
- **ABC, FIP (notched)**

**Axes:**
- **N, cycles** (10^4 to 10^6)
- **S, MPa** (0 to 500)

**Legend:***
- Red line: ABC, FIP (un-notched)
- Black line: Linear-Elastic
- Green line: Neuber
- Blue dashed line: ABC, FIP (notched)
Summary and Conclusions

• ABC uses a multiscale multicomponent formulation rooted in micromechanics to predict material behavior

• ABC can predicted notch sensitivity of notched devices, giving information of geometric effects and statistics

• Goal is that device designers can optimize microstructure and geometry concurrently
Constitutive Modeling

Simple Partition

- Archetype A = matrix
- Archetype B = Inclusion
- Partition 1 = matrix
- Partition 2 = matrix inclusion

Realistic Partition

- Archetype A = matrix
- Archetype B = carbide
- Archetype C = oxide
- Archetype D = damaged matrix/oxide interphase
- Partition 1 = matrix
- Partition 2 = matrix carbide
- Partition 3 = matrix oxide
- Partition 4 = matrix oxide interphase

Eshelby’s Problem

Homogenization with Eigenstrain $\epsilon^*$

$$L_1(\epsilon^0 + S\epsilon^*) = L_0(\epsilon^0 + S\epsilon^* - \epsilon^*)$$

Where $L_0$ and $L_1$ are stiffness tensors, $S$, Eshelby’s tensor and $\epsilon^0$ the applied strain.

Solving for Eigenstrain $\epsilon^*$ gives:

$$\epsilon^* = -[(L_1 - L_0)S + L_0]^{-1}(L_1 - L_0)\epsilon^0$$

If the inclusion strain $\epsilon_1$ is given by:

$$\epsilon_1 = \epsilon^0 + S\epsilon^*$$

Then the inclusion strain is

$$\epsilon_1 = (I + SL_0^{-1}(L_1 - L_0))\epsilon^0$$

This maps the applied strain to the inclusion strain based on the material properties of the matrix and inclusion and Eshelby’s tensor.

For an arbitrary complex problem a region around the inclusions ($\tau$) can be considered with a material properties $\hat{L}$ and applied strain $\hat{\epsilon}$, then the inclusion strain is

$$\epsilon_\tau = (I + S\tau \hat{L}^{-1}(\tau - \hat{L}))\hat{\epsilon}$$

Different assumptions for $\hat{L}$ and $\hat{\epsilon}$ yield many popular micromechanics models:

- Dilute Model : $\hat{L} = L_0; \hat{\epsilon} = \bar{\epsilon}$
- Mori-Tanaka : $\hat{L} = L_0; \hat{\epsilon} = \bar{\epsilon}_0$
- Self Consistent : $\hat{L} = \bar{L}; \hat{\epsilon} = \bar{\epsilon}$