McCormick

Northwestern Engineering

# Archetype-Blending Multiscale Continuum Method

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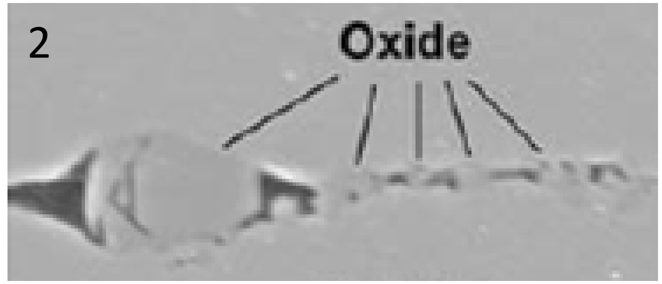
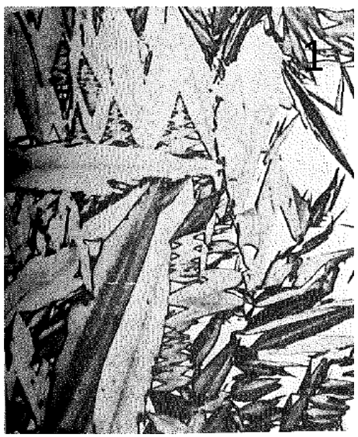
# Outline

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

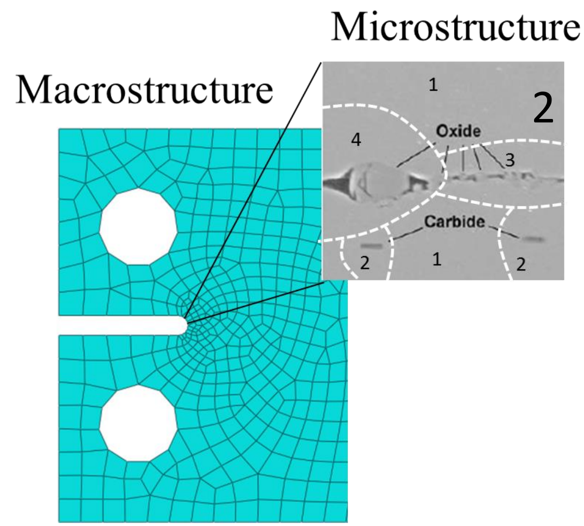
# Motivation and Background

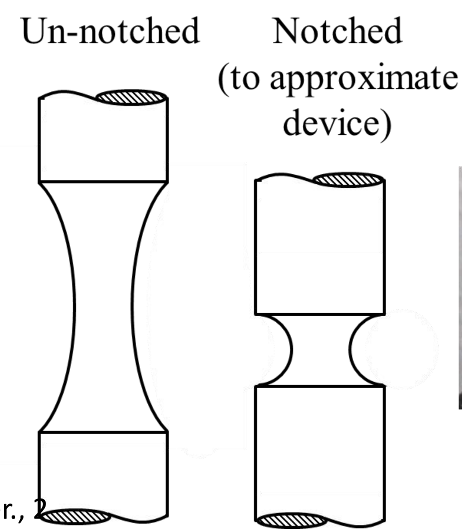


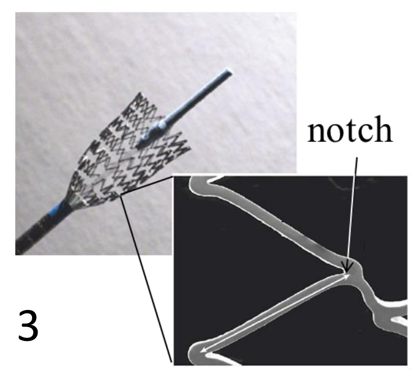




Microstructure

Macrostructure



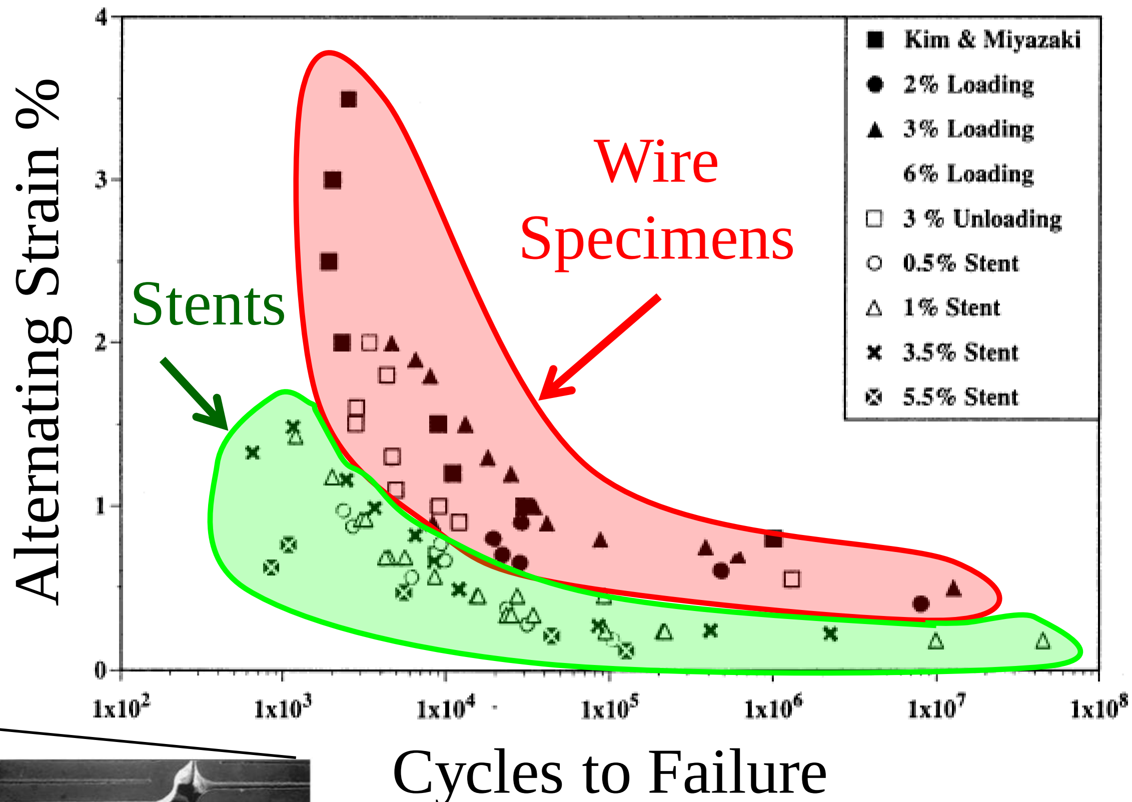


1 Porter, Easterling,2004

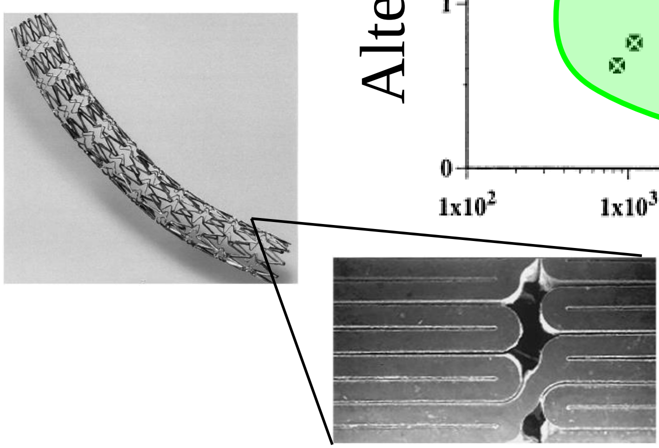
2 Toro et. al, J. Mater. Eng. Perform 2009

3 Pelton, et al J. Mech. Behav. Biomed Mater., 2

# Fatigue in Biomedical Stents

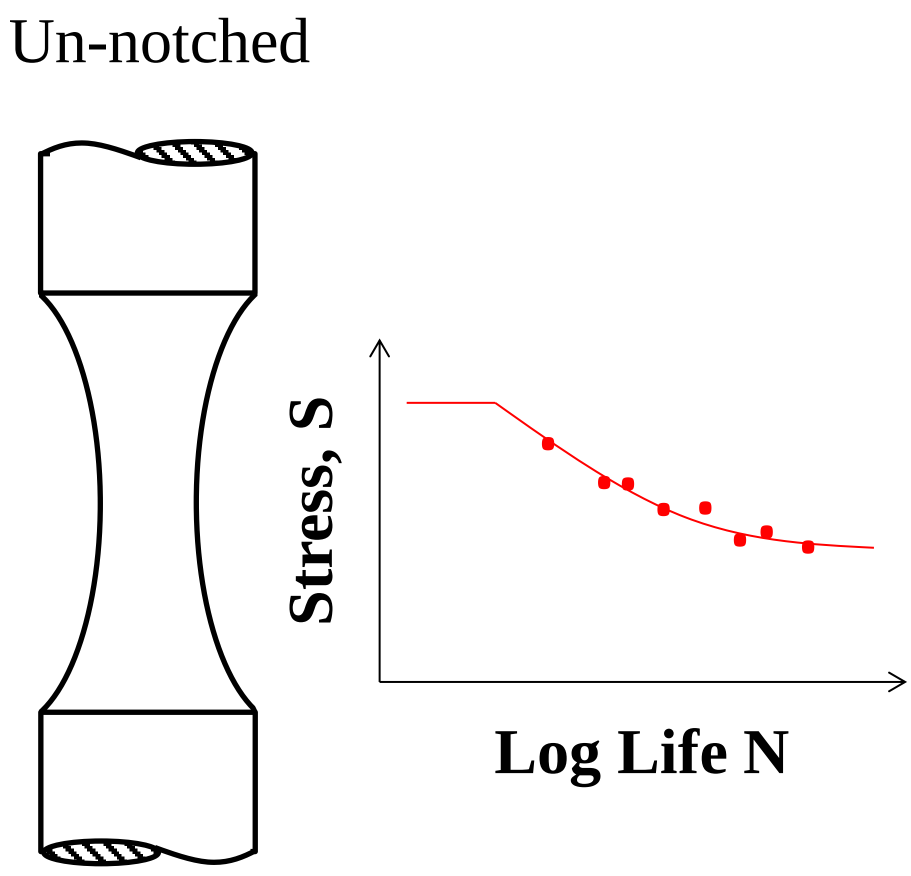


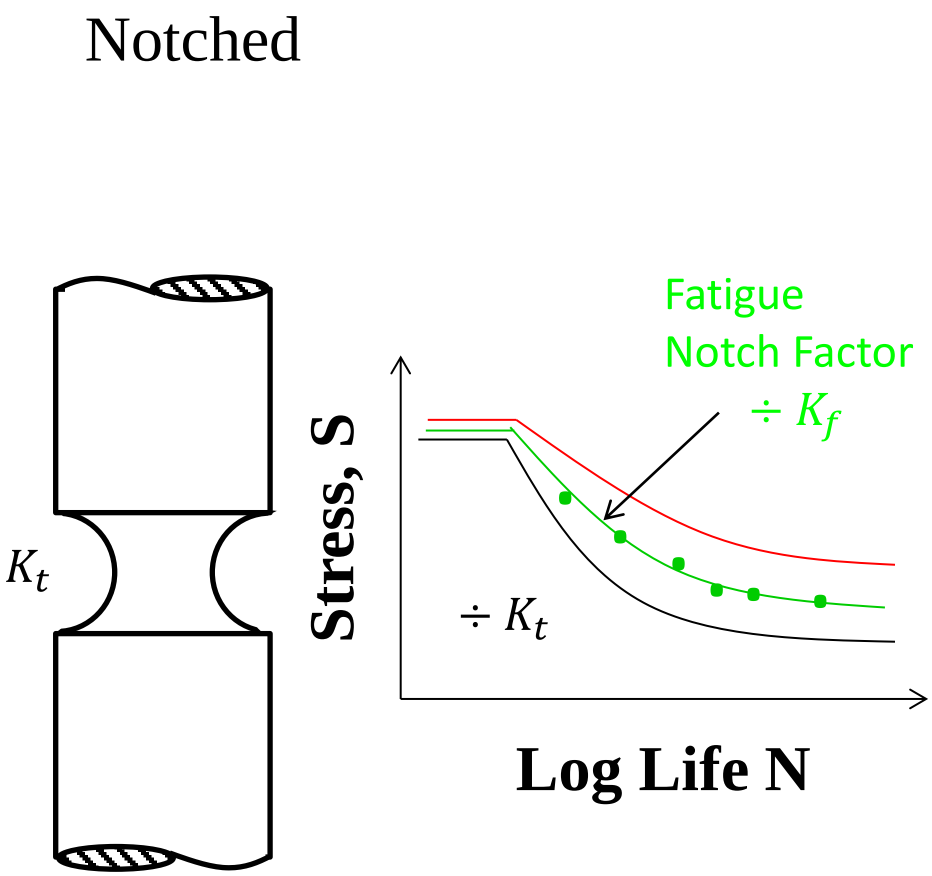

Stent



Duerig, T., A. Pelton, and D. Stöckel, *An overview of nitinol medical applications.* Materials Science and Engineering: A, 1999.

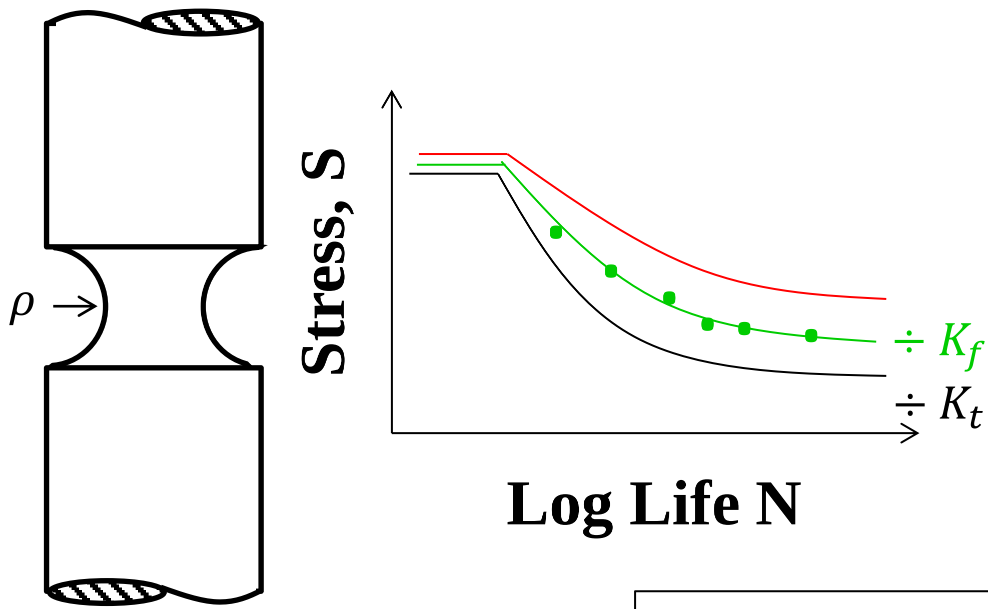
# Notch Effects



# Neuber's Equation

Notched




Neuber's Equation

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

Non-linear

Material dependent

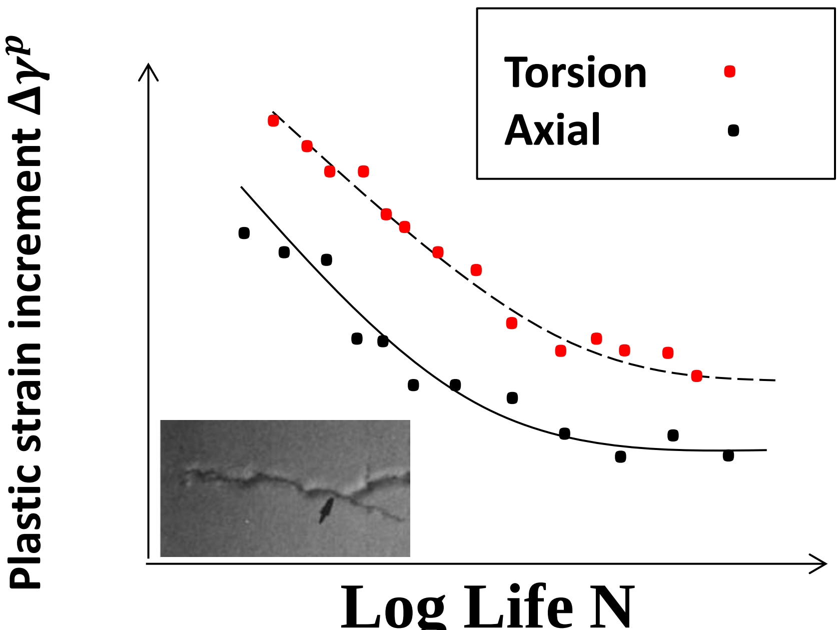
Non-linear material dependent behavior indicates microstructural dependence

Schijve, Fatigue of Structures and Materials, 2001

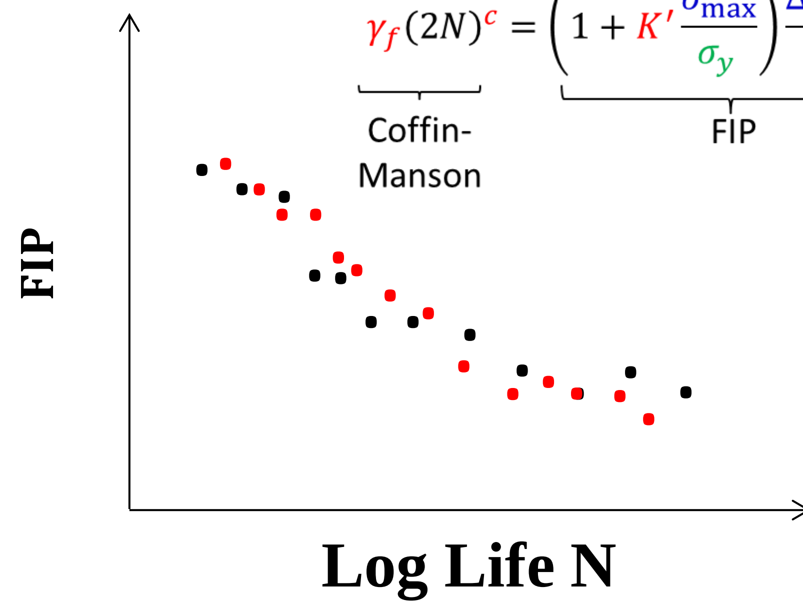
# Computational Fatigue

- Fatemi-Socie in 1988 proposed a **f**atigue **i**ndicating **p**arameter (**FIP**) to account for discrepancies in $\epsilon$-N curves due to loading condition

Empirical Constant (red)
Material Parameter (green)
From FEM/Experiment (blue)




$$\underbrace{\gamma_f (2N)^c}_{\text{Coffin-Manson}} = \underbrace{\left(1 + K' \frac{\sigma^n_{\max}}{\sigma_y}\right)\frac{\Delta\gamma^p_{\max}}{2}}_{\text{FIP}}$$




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
- Microstrucurally Small Cracks ($N_{MSC}$) : growth of crack from incubation size $a_i$, such that $a_i < a < k\text{GS}$, where $k$ is (1-3) and GS 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

$$N_{Total} = N_{Inc.} + N_{MSC} + N_{LC}$$

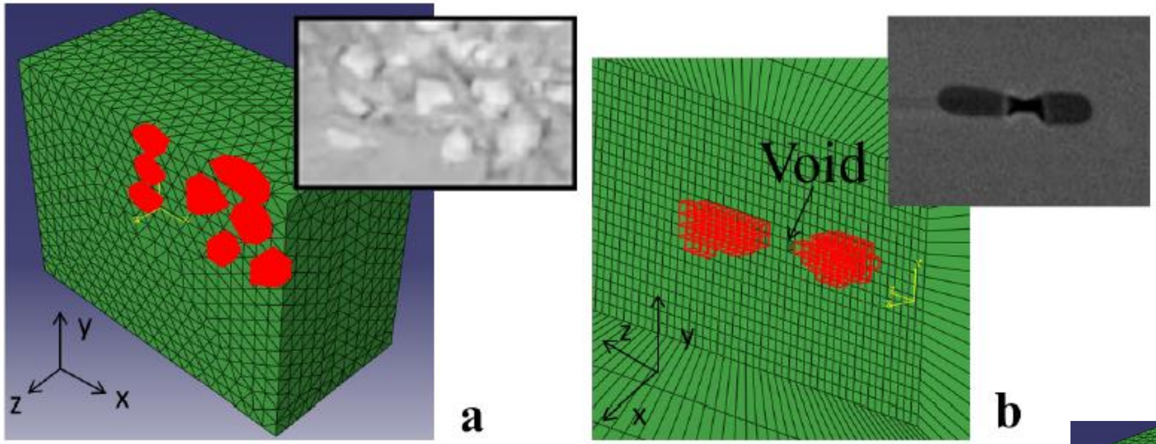
- The following work will address only $N_{Inc.}$ as it accounts for a large % of fatigue life for many alloys

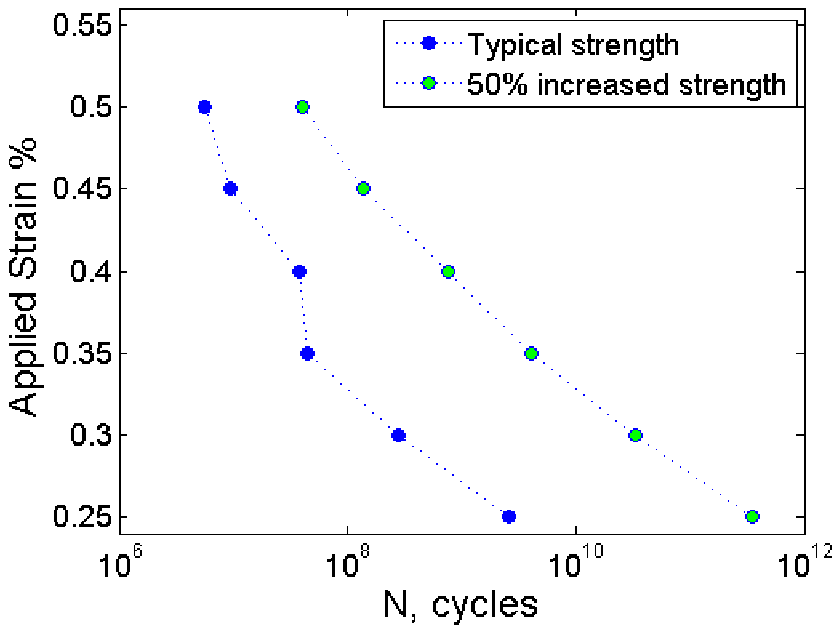
- The ABC theory will be able to model the $N_{MSC}$ and $N_{LC}$ regimes by:
  - Studying several (5-10) initial cycles and determining $N_{Inc.}$ from a FIP
  - Using this as an initial state for explicit modeling of $N_{MSC}$ and $N_{LC}$
  - $N_{MSC}$ region could be considered 1 element (kGS = 1 element) and growth modeled with methods such as XFEM[1]
  - 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

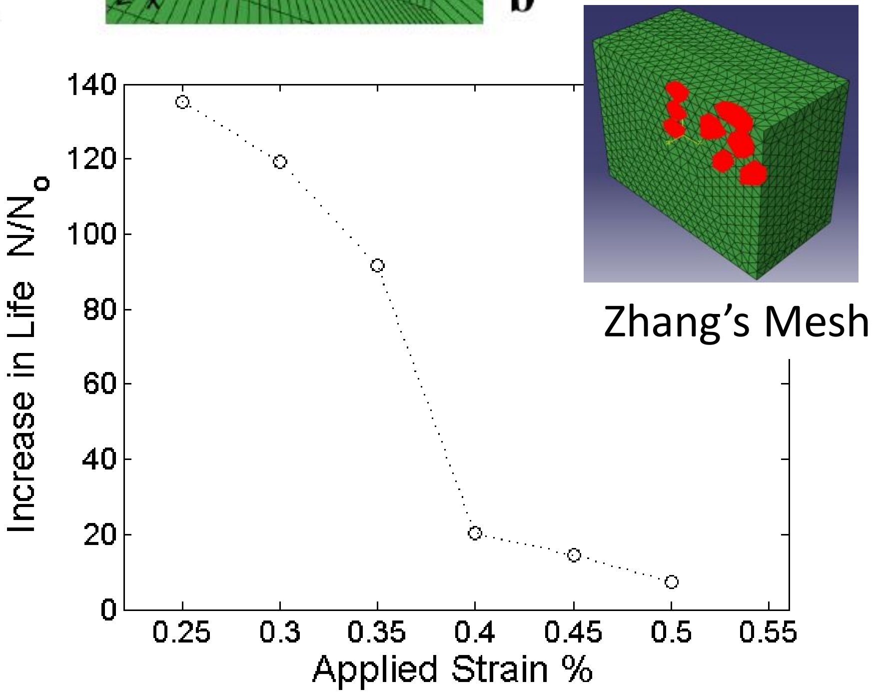
1 Menouillard, Thomas, et al. "Time dependent crack tip enrichment for dynamic crack propagation." Int. J. of Frac.162.1-2 (2010): 33-49.

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

# Direct Numerical Simulation of FIP



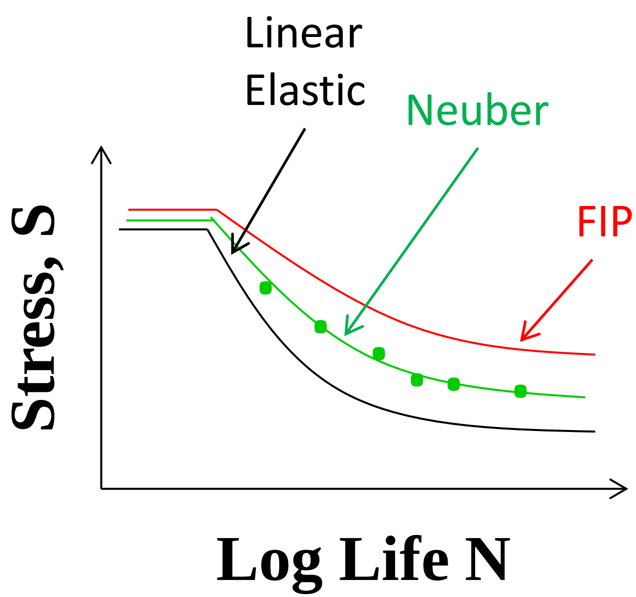




Zhang's Mesh

Zhang et al. Eng. Fract,Mech, 2009

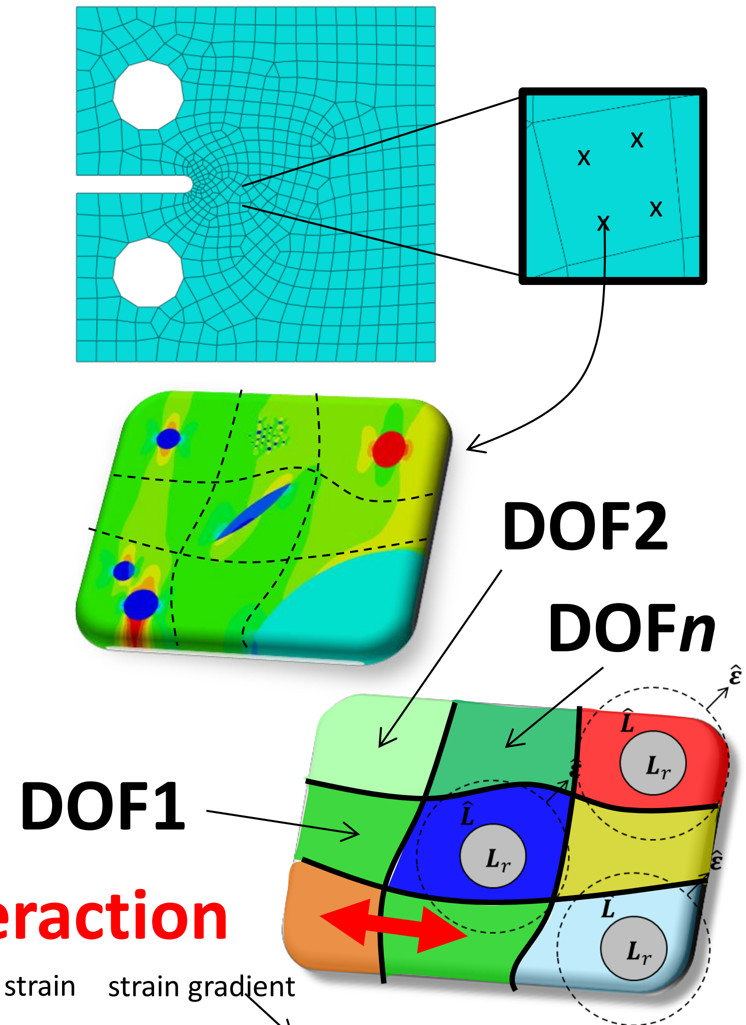
# Fatigue Theory Summary

- 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



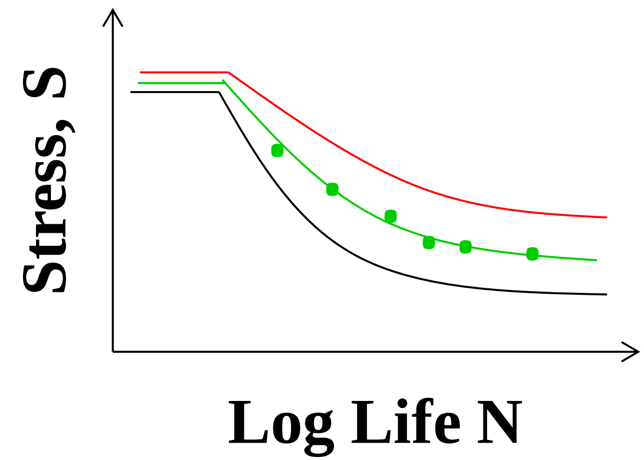

Intrinsic stress, relative stress, relative strain, strain gradient

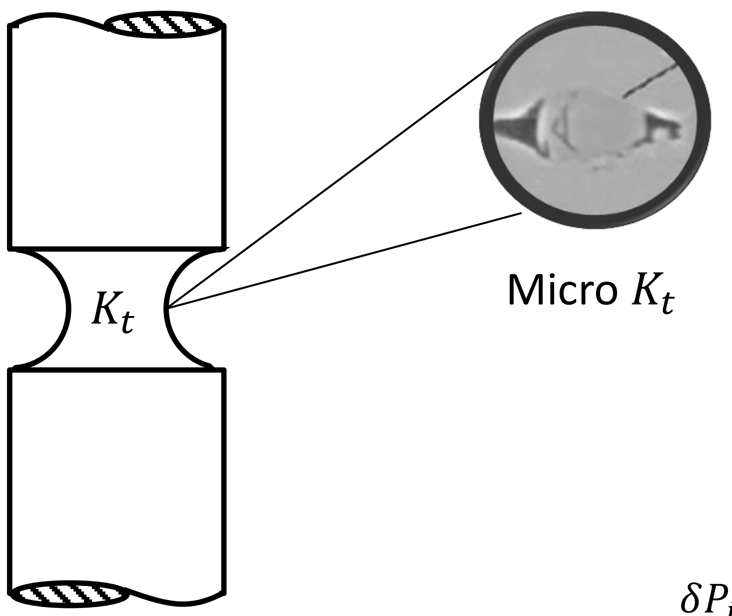
$$\delta P_{int} = \int_{\Omega} \left( \boldsymbol{\sigma} : \delta \widehat{\boldsymbol{L}} + \boldsymbol{\sigma\sigma} \vdots \delta \widehat{\boldsymbol{L}} \nabla + \boldsymbol{s}^n : \delta \boldsymbol{\Lambda}^n + \boldsymbol{ss}^n \vdots \delta \boldsymbol{\Lambda}^n \nabla \right) d\Omega$$

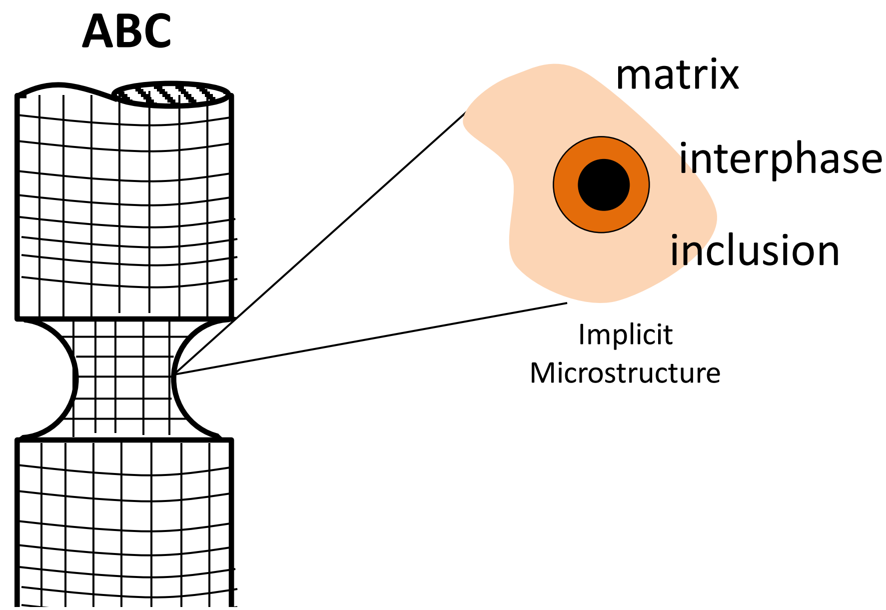
Elkhordary et al., Comput. Methods Appl. Mech. Engrg., 2013

# Notched Fatigue and ABC

- Non-linear reduction in S-N curve is :
  - Material dependent
  - A function on macroscale strain gradients[1]
  - A function of microscale strain gradients[1]



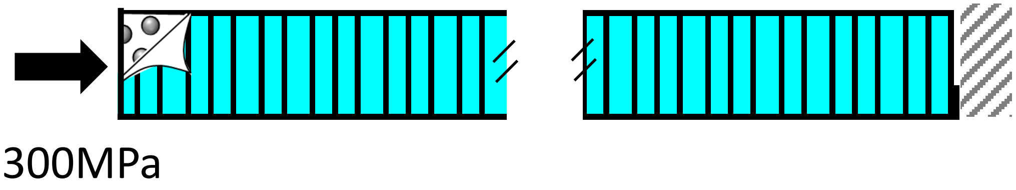




$$\delta P_{int} = \int_{\Omega} \left(\boldsymbol{\sigma}: \delta\hat{\mathbf{L}} + \sigma\sigma \,\vdots\, \delta\hat{\mathbf{L}}\nabla + \mathbf{s}^n: \delta\Lambda^n + \mathbf{ss}^n \,\vdots\, \delta\boldsymbol{\Lambda}^n\nabla\right) d\Omega$$

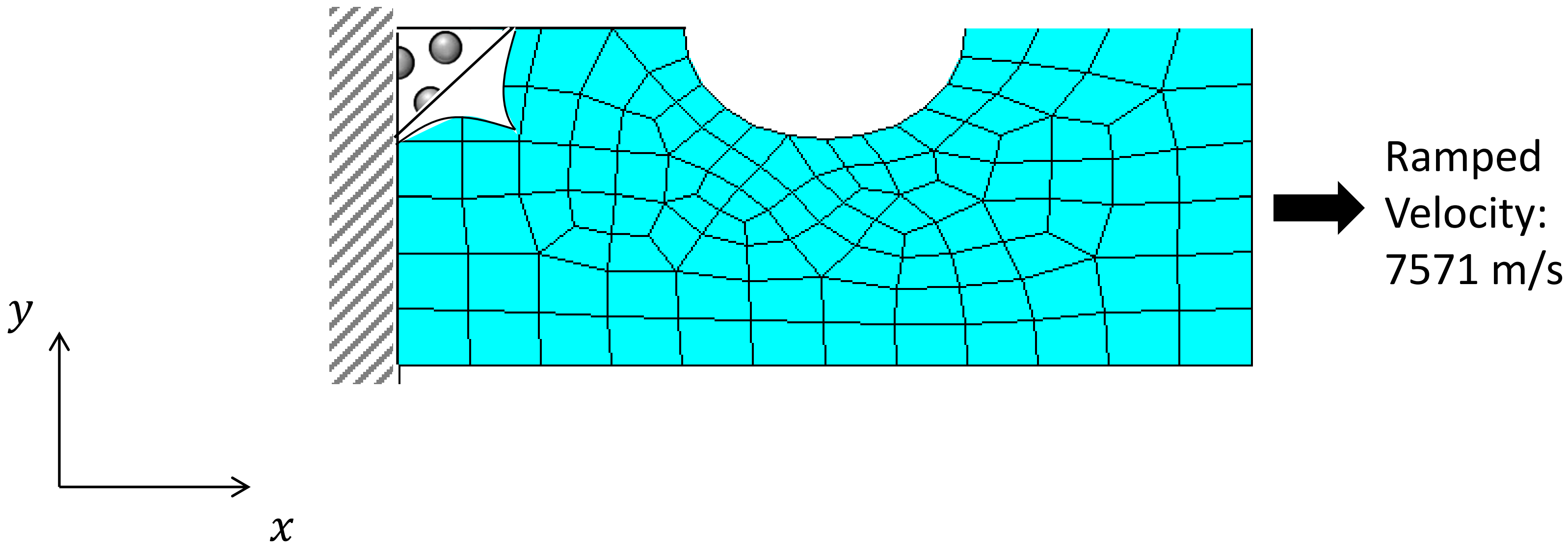
1 McDowell, Mat. Sci. Eng. A, 2007

# Models

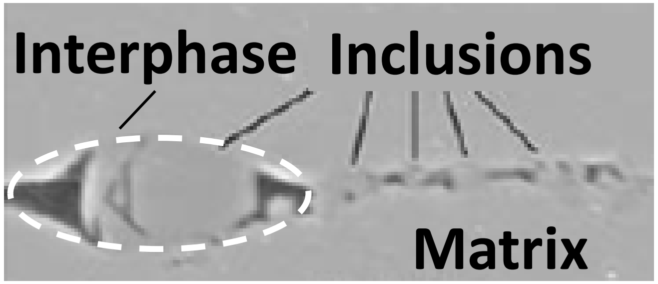
10% volume fraction




1% volume fraction



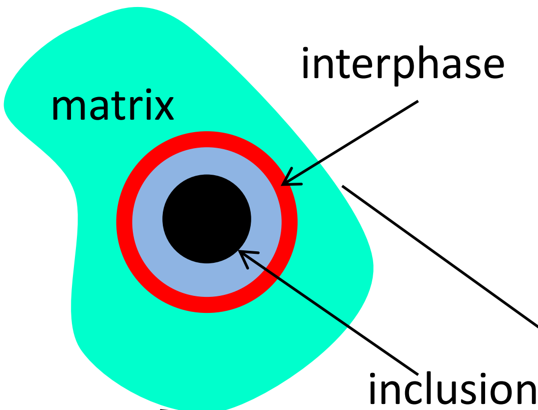
# Implicit Microstructure

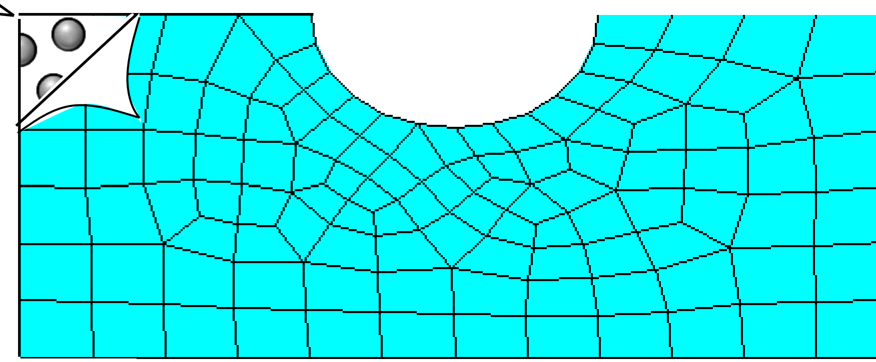



**Matrix**: Young's Modulus: 200 GPa
Yield Strength : 250 MPa

**Interphase**: Young's Modulus: 200 GPa
Yield Strength : 250 MPa

**Inclusion**: Young's Modulus: 2000 GPa
Linear Elastic

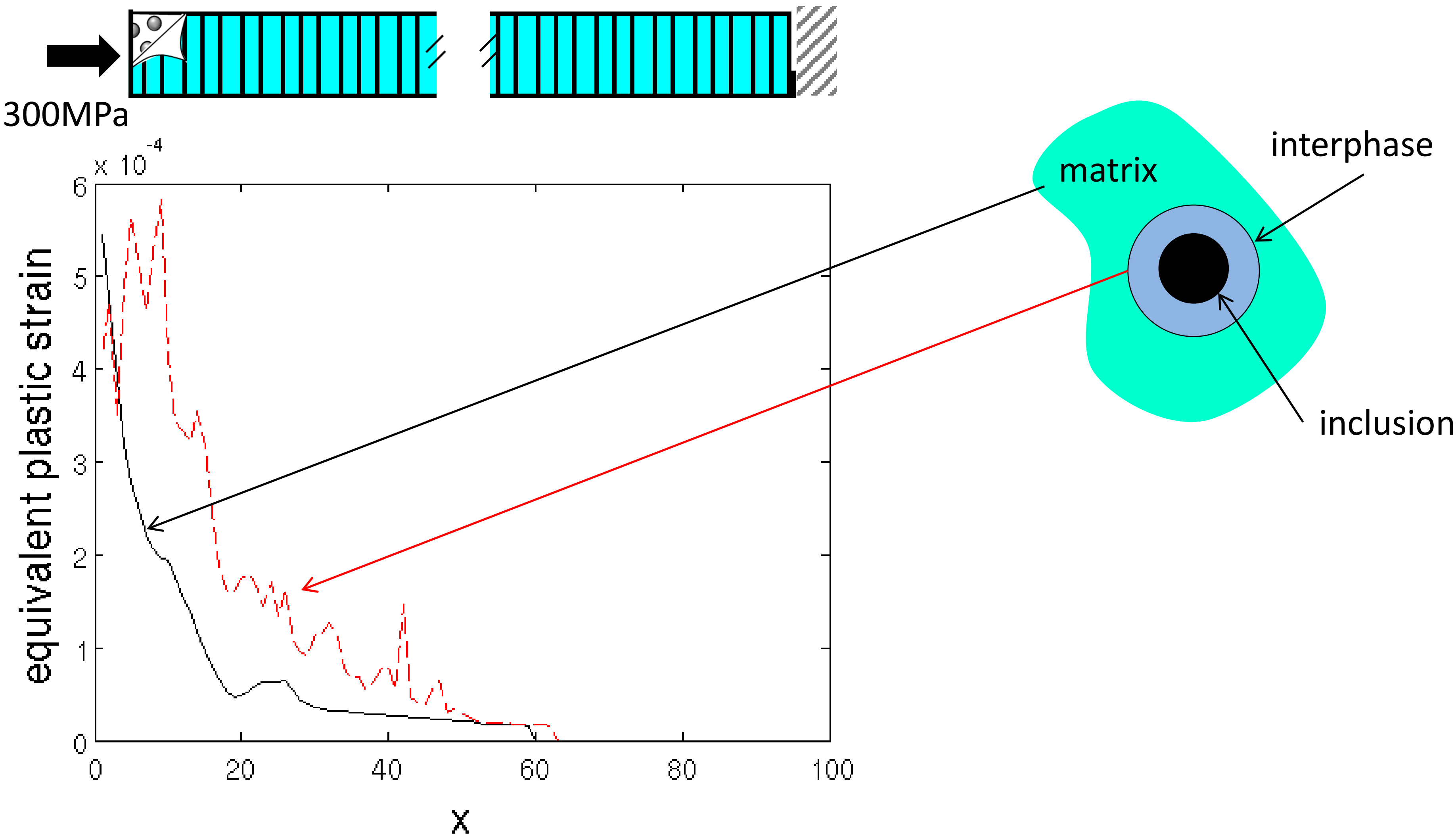


| | | |
|---|---|---|
| Degree-of-Freedom 1 | $\varepsilon^1$ | Matrix |
| Degree-of-Freedom 2 | $\varepsilon^2$ | Interphase |
| | $\mathfrak{E}(\varepsilon^2)$ | Inclusion |

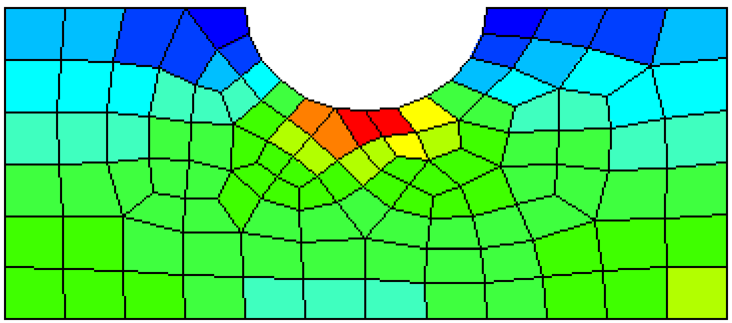
$\mathfrak{E}$ = mapping of strain using Eshelby's solution

# Microplasticity

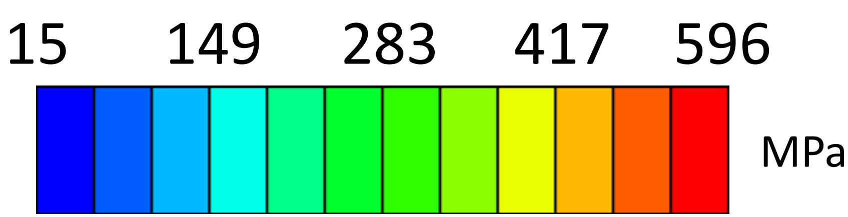


# Response of Notched Sample

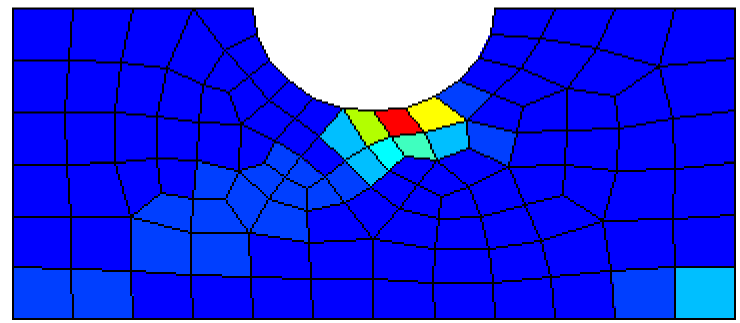
## Linear Elastic Macro Stress

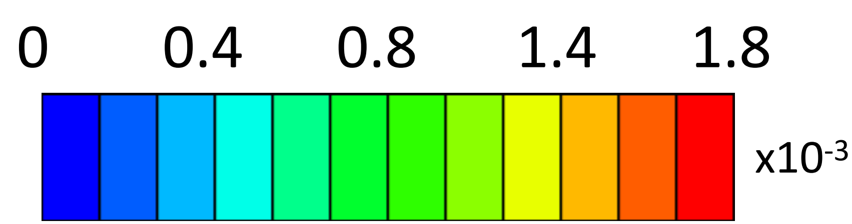


Stress w/o notch is 300 MPa,
$K_t \approx 2$

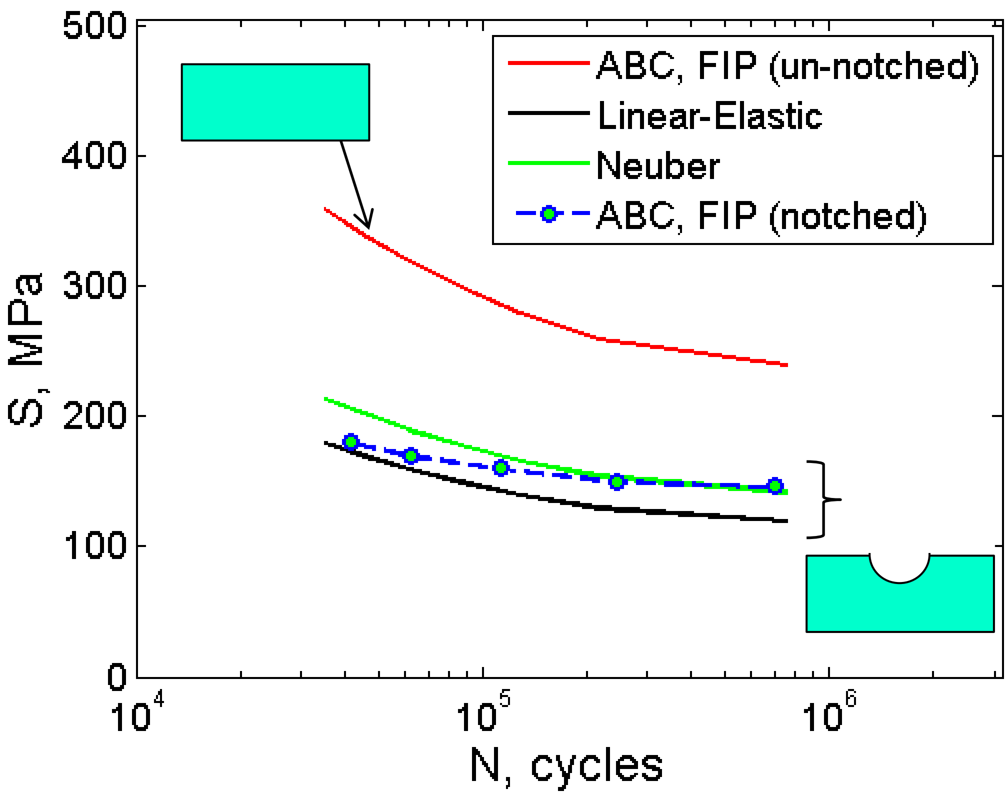



## Equivalent Plastic Interphase Strain





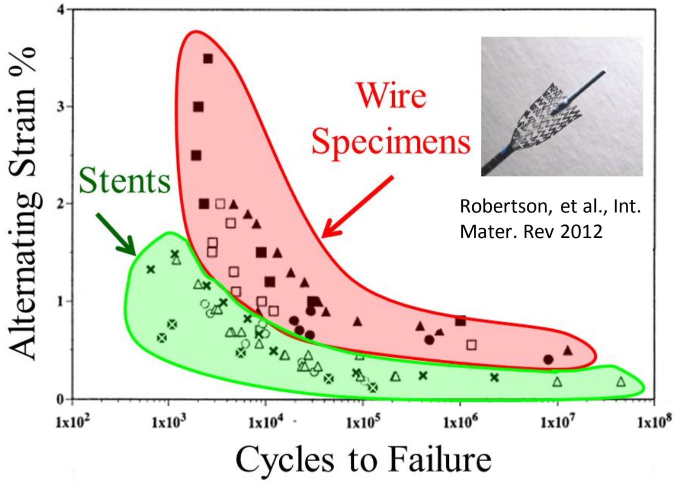
# Notched Sample Fatigue Prediction

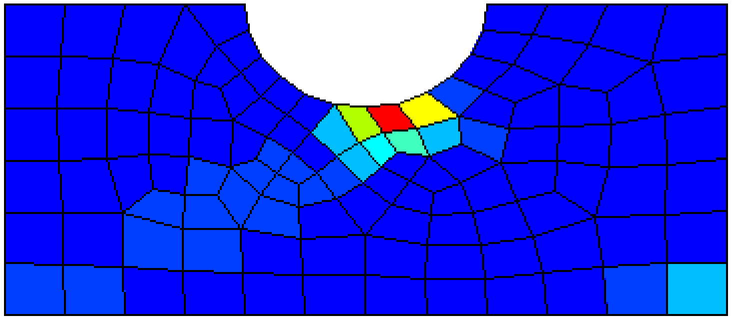


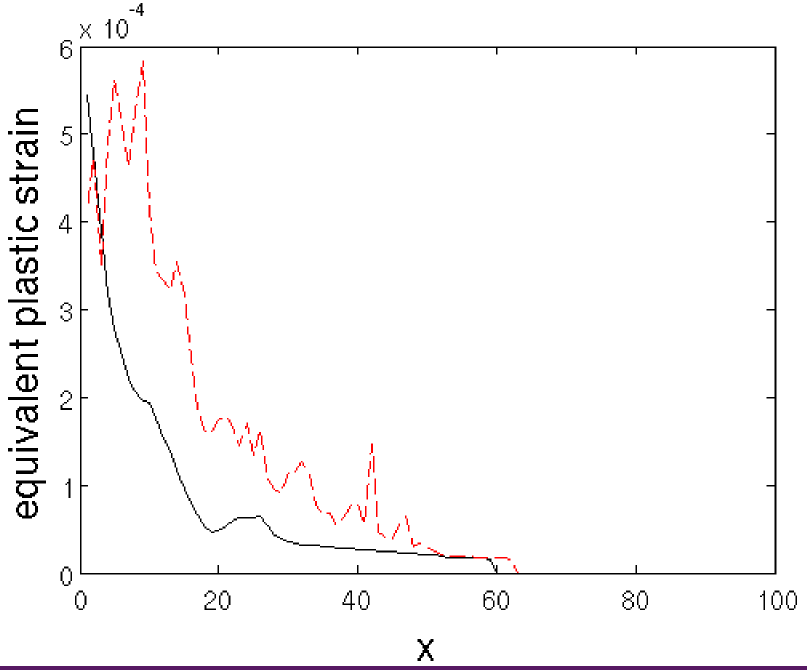
# Summary and Conclusions

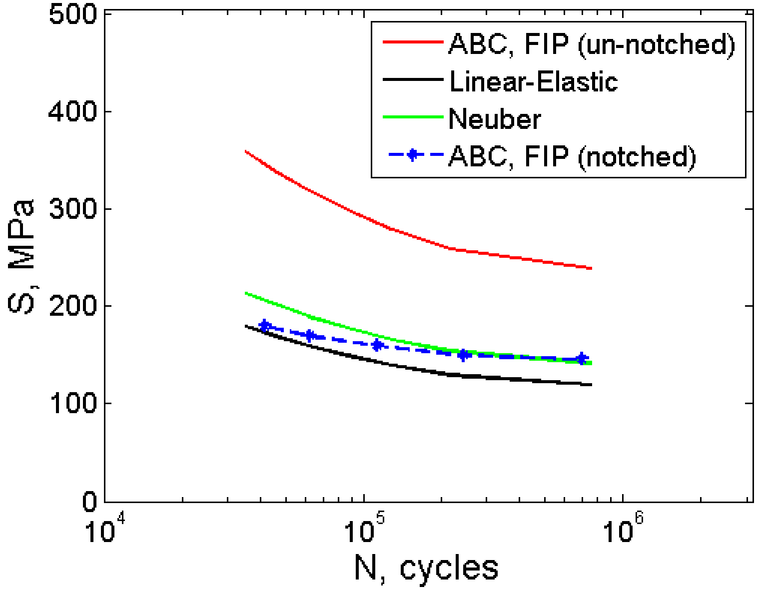
- ABC uses a multiscale multicomponent formulation rooted in micromechanics to predict material behavior
- ABC can predicted notch sensitivity of notched devices, giving information of geometric effects and statistics
- Goal is that device designers can optimize microstructure and geometry concurrently

# Questions / Comments



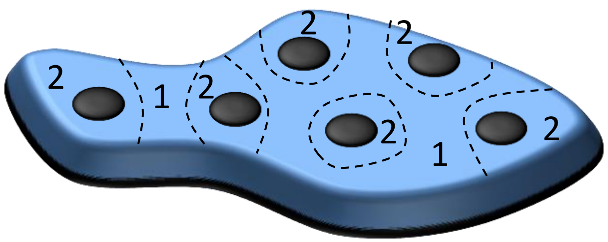


# Backup

# Constitutive Modeling

## Simple Partition



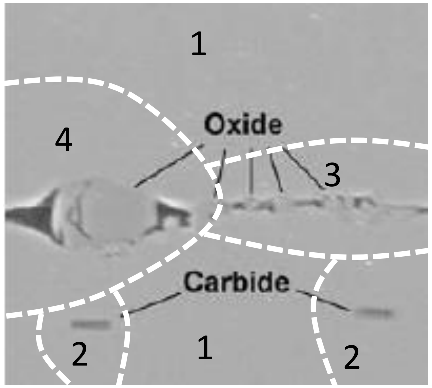

Archetype A = matrix

Archetype B = Inclusion

Partition 1 = matrix

Partition 2 = matrix
inclusion

## Realistic Partition




Partition 1 = matrix

Partition 2 = matrix
carbide

Partition 3 = matrix
oxide

Partition 4 = matrix
oxide
interphase

Archetype A = matrix

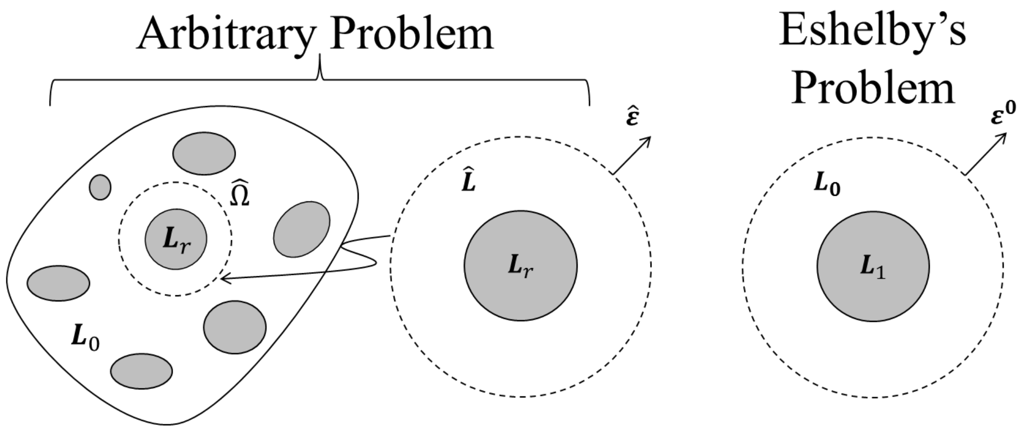
Archetype B = carbide

Archetype C = oxide

Archetype D = damaged matrix/oxide interphase

Toro et. al, J. Mater. Eng. Perform Volume 18(5–6) August 2009

# Eshelby's Problem




Then the inclusion strain is

$$\boldsymbol{\varepsilon_1} = \{\boldsymbol{I} + \boldsymbol{S}\boldsymbol{L_0^{-1}}(\boldsymbol{L_1} - \boldsymbol{L_0})\}\boldsymbol{\varepsilon^0}$$

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

Homogenization with Eigenstrain $\varepsilon^*$

$$\boldsymbol{L_1}(\boldsymbol{\varepsilon^0} + \boldsymbol{S}\boldsymbol{\varepsilon}^*) = \boldsymbol{L_0}(\boldsymbol{\varepsilon^0} + \boldsymbol{S}\boldsymbol{\varepsilon}^* - \boldsymbol{\varepsilon}^*)$$

Where $\boldsymbol{L_0}$ and $\boldsymbol{L_1}$ are stiffness tensors, $\boldsymbol{S}$ , Eshelby's tensor and $\boldsymbol{\varepsilon^0}$ the applied strain

Solving for Eigenstrain $\varepsilon^*$ gives :

$$\boldsymbol{\varepsilon}^* = -[(\boldsymbol{L_1} - \boldsymbol{L_0})\boldsymbol{S} + \boldsymbol{L}_0)]^{-1}(\boldsymbol{L_1} - \boldsymbol{L_0})\boldsymbol{\varepsilon^0}$$

If the inclusion strain $\varepsilon_1$ is given by:

$$\boldsymbol{\varepsilon_1} = \boldsymbol{\varepsilon^0} + \boldsymbol{S}\boldsymbol{\varepsilon}^*$$

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

$$\boldsymbol{\varepsilon_r} = \{\boldsymbol{I} + \boldsymbol{S_r}\hat{\boldsymbol{L}}^{-1}(\boldsymbol{L_r} - \hat{\boldsymbol{L}})\}\hat{\boldsymbol{\varepsilon}}$$

Different assumptions for $\hat{\boldsymbol{L}}$ and $\hat{\boldsymbol{\varepsilon}}$ yield many popular micromechanics models

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