Multiresolution Probabilistic Nano Mechanics and Materials From Validation to Prediction

In particular for:
Reliability Prediction in Heterogeneous Materials and Materials Design
Fusion with Product Design and Manufacturing

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Overview

• Main contributions of Multiresolution Probabilistic Nano Mechanics and Materials.

• Overview of Digital 3D Materials Design and Multi-Material Systems.

• Materials which fail over multiple length and time scales.

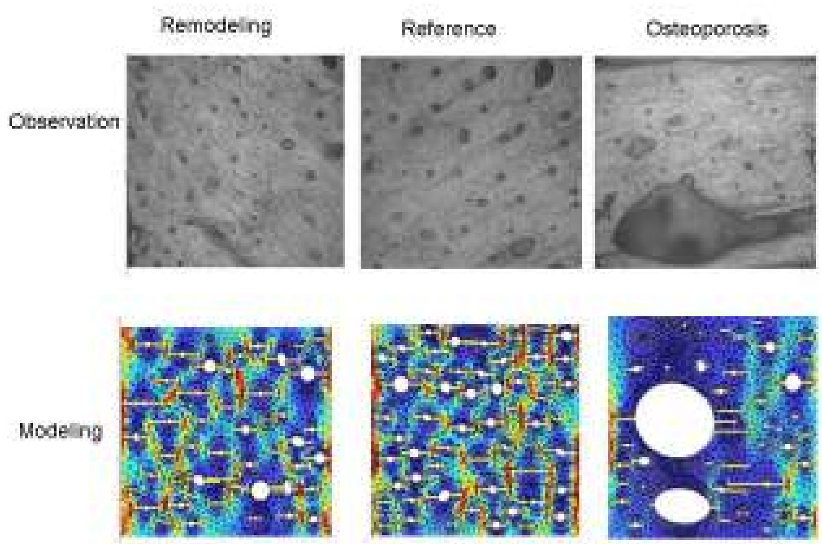
• Simulation of Probabilistic Science-based Predictive Models for constitutive equations, materials instability, and equation of states.

• Multiresolution statistical continuum theory for nano/microstructural materials.

• Comparison with traditional continuum.

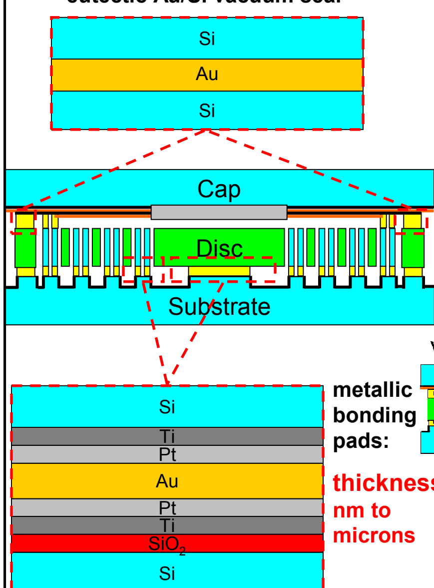
• The Future: Probabilistic Computational Science-based Mathematical Framework; verification and validation through limited experiments; and LIFE-CYCLED MATERIALS DESIGN for products design and manufacturing through the use of Petaflop Computing.

Microstructure Evolution of the Cortical Bone (Elisa Budyn)



ASC Focus: Structural Integrity of MicroSystems

• **eutectic Au/Si vacuum seal**

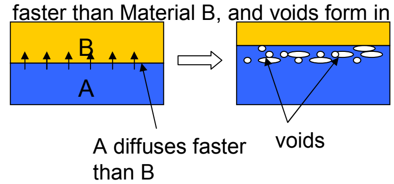


metallic bonding pads:

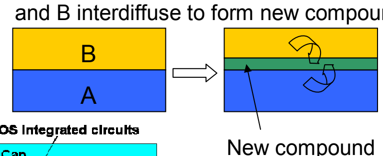
thickness: **nm to microns**

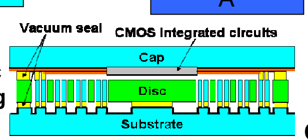
VLSI manufacturing technique

• **Kirkendall effect** – Material A diffuses faster than Material B, and voids form in

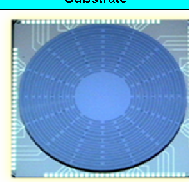


• **Compound formation** – Materials A and B interdiffuse to form new compound.





Courtesy of Boeing

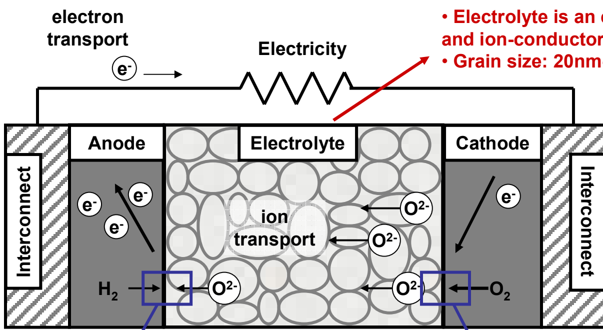


MEMS vibratory mechanical gyros offer to provide longer life and reliability with much greater performance per unit mass than either with very low power, e.g.1 cc, and 5mw.

How Do Fuel Cells Work

Electrons are transported through external circuit (Interconnects) delivering electric power.

- **Electrolyte is an electron-insulator and ion-conductor.**
- **Grain size: 20nm-few μm**



At the anode, hydrogen is oxidized into water and electrons.

$$H_2 + O^{2-} \rightarrow H_2O + 2e^-$$

Oxygen ions are transported through an ion conducting electrolyte

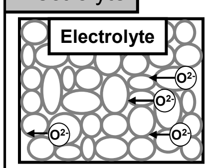
At the cathode, oxygen is reduced to oxygen ions.

$$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$$

Anode		Cathode
generate **electrons**	electron transport via interconnect →	consume **electrons**
consume **oxygen ions**	← oxygen ion tranport via electrolyte	generate **oxygen ions**

Energy Generating Devices: Fuel Cells and Thermoelectric Materials

Electrolyte



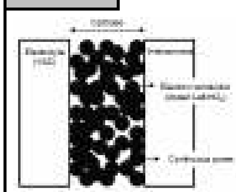
Desired properties
- High ionic conductivity
- Negligible electronic conductivity
- Gas-tightness
- High strength and toughness

Design parameters
- Grain size
- Dopant level

Nanosized grains increase conductivity, and thus efficiency.

Adding alumina particles increases toughness without much degrading efficiency.

Cathode

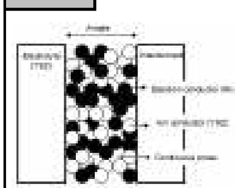


Desired properties
- High gas diffussivity
- High electrical conductivity
- High catalytic activity
- Large reaction site

Design parameters
- Volume fraction
- Partcle size

Nanoparticles generate more reaction site, and thus increase efficiency.

Anode

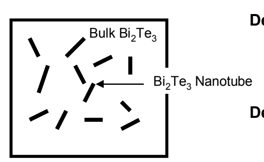


Desired properties
- High gas diffussivity
- High electrical conductivity
- High catalytic activity
- Large reaction site

Design parameters
- Volume fraction
- Particle size

Nanoparticles generate more reaction site, and thus increase efficiency.

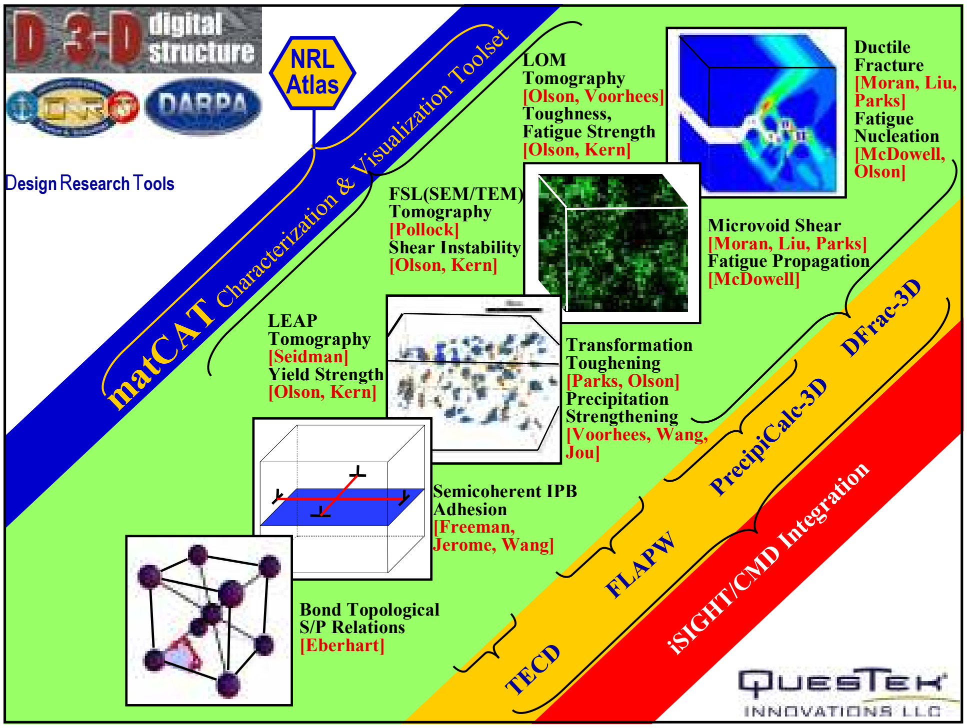
Thermoelectric materials



Desired properties
- High electrical conductivity
- Low thermal conductivity

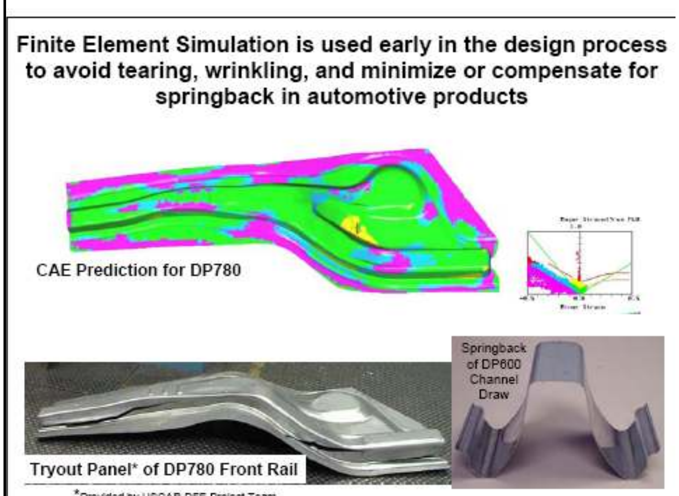
Design parameters
- Volume fraction
- Particle size

Nanoparticles decrease thermal conductivity, and thus increase efficiency.



Forming Limit Diagram (FLD) not Application to AHSS

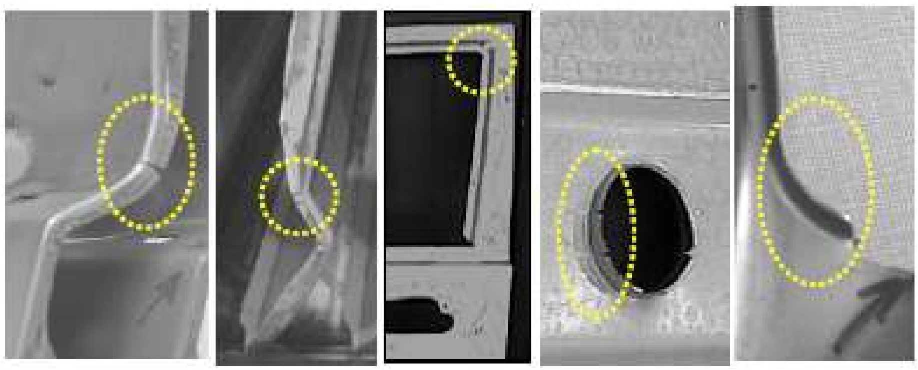
"Local Formability Issue One" - Shear Fracture at Tight Radius in the Die



Forming Limit Diagram (FLD) says it's safe (no red spots in the color contour, most are green in the fracture area), but the experiments showed differently.

How to predict this based on microstructure?

"Local Formability Issue Two" - Edged Cracking in Stretch Flanging

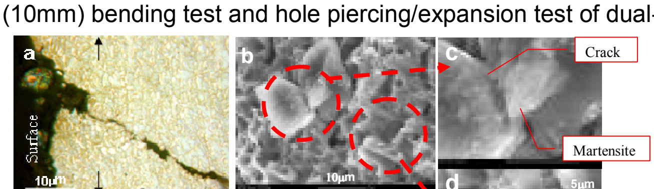


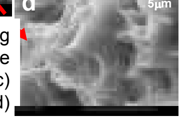
Edge cracking in stretch flanging occurred before predicted value from forming limit diagram.

Taken from Bhattacharya's slide at the NSF Workshop, Oct., 2006

Fractured surfaces of AHSS DP780

Small-radius (10mm) bending test and hole piercing/expansion test of dual-phase DP780





Fractured surfaces of DP780. (a) a crack passing through ferrite and deflected by martensite particles (2% nital/30s); (b) a fractured surface, (c) the crack penetrates a martensite phase; (d) ductile fracture in ferrite phase.

(courtesy of Xin Wu, Wayne State Univ)

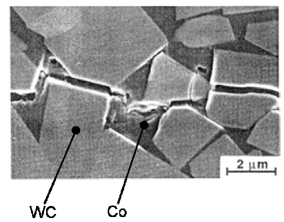
Crack took a path that is affected by the martensite particle distribution pattern (a), and both ductile fracture within ferrite and brittle fracture within martensite were seen (b-d).

Interfacial fracture at phase boundary was not clearly identified at this stage.
In the case of small radius bending the results also showed that surface quality has an important impact to shear fracture.

The crack attempted to propagate along 45º to the outer surface and in order to satisfy this orientation within a narrow bent it developed a zig-zag path. The issues related to microstructure and fracture of AHSS

WC Co Composite

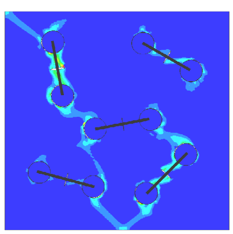
- Ductile Reinforced Brittle Composite WC-Co
- Brittle phase is WC ~85% by volume
  - *Very strong but brittle*
- Ductile phase is Co ~15% by volume
  - *Very ductile but low strength*



- Composite system combines the strength of WC and the toughness of Co

- Aerospace, munitions, sports, automobile, home appliances, **cutting tools**, metal forming tools, mining tools and wear resistance surfaces

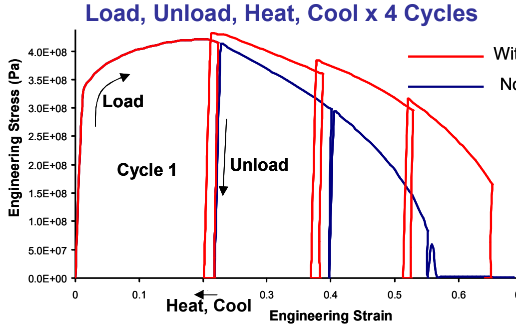
Self Healing Composites



S.M.A. Fiber

- Shape Memory Alloy Fibers embedded in a matrix material
- Cracks are bridged by the fibers
- Fibers elongate as cracks open
- HEAT: fibers regain original shape through phase transformation
- Crack faces are pulled together by anchored fibers

Load, Unload, Heat, Cool x 4 Cycles

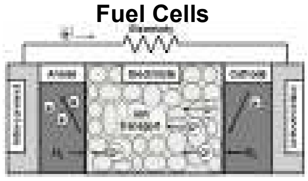


- Several loading and heating cycles
- Composite retains more strength and ductility

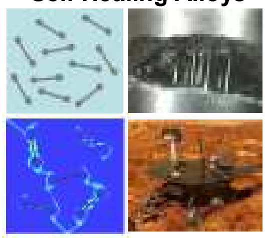
Nano/Micro Materials & Devices Design

GOAL: A General Multiscale Design Framework For Heterogeneous Materials to Maximize Performance and Durability of a System

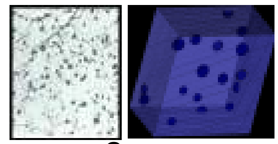
Fuel Cells



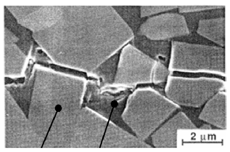
Self Healing Alloys



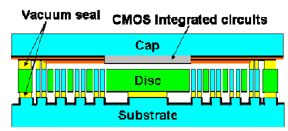
High Strength Alloys



Composites

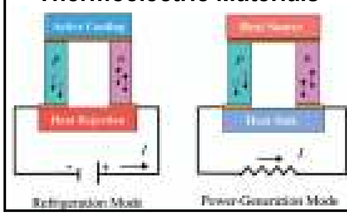


Gyroscopes

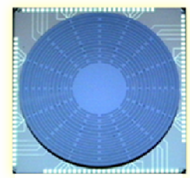


Nano/Micro Scale Failure

Thermoelectric Materials



Too large for first principles approaches
Too small for conventional FEA
• Approach: A Multiresolution FE theory



Courtesy of Boeing

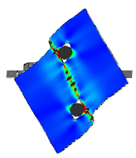
Thermoelectric Materials, Phenomena, and Applications: A Bird's Eye View, Terry M.Tritt and M.A. Subramanian, MRS Bull., 2006, 31(3), 188

Failure & Performance in Micro/Nano Materials Systems

- **Often involve thermal-mechanical-electrical-mass diffusion effects**
- **Can occur at different scales simultaneously or successively**
- **Scale at which material degradation occurs strongly effects performance**
- **Models must capture the magnitude and scale of material degradation**

Main Contributions: From Validation to Prediction

Computational Experiments	Multiresolution Constitutive Equations	Multiresolution Continuum Equations	Predict Performance



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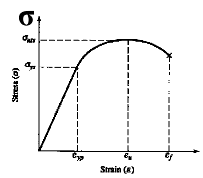

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σ

$\boxed{\beta^n, \overline{\beta}^n}$

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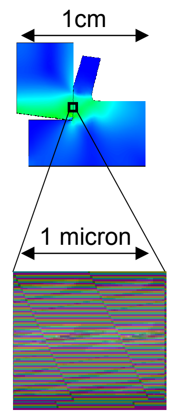
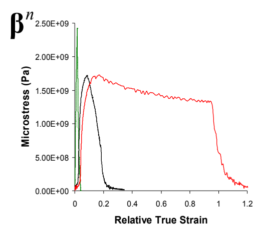


1. Derive constitutive relationships from computational simulations

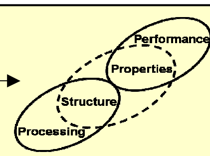


2. Include microstresses which capture inhomogeneous deformation

Introduction to Nano/Micro Materials Design

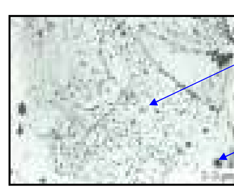
- ❑ Goal: In material design we relate material properties to microstructure

Missing link in material design →



- ❑ Macroscale properties controlled by shear banding, localization and fracture behavior
- ❑ These phenomena are activated by microscale features e.g. inclusions
- ❑ Macroscale specimens cannot be explicitly modeled (e.g. MD or QM with inclusions, micro cracks, etc) - prohibitively expensive

Design microstructure of steels to maximize strength and toughness

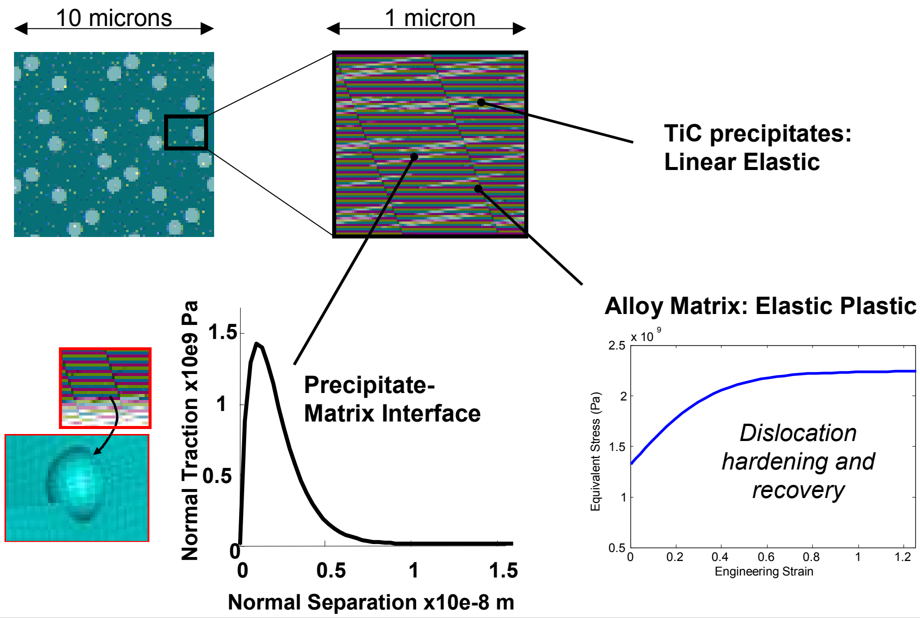


Secondary particles
(0.01-0.1 micron)

Primary Particles
(1 micron)

So how do we preserve the small scale description?

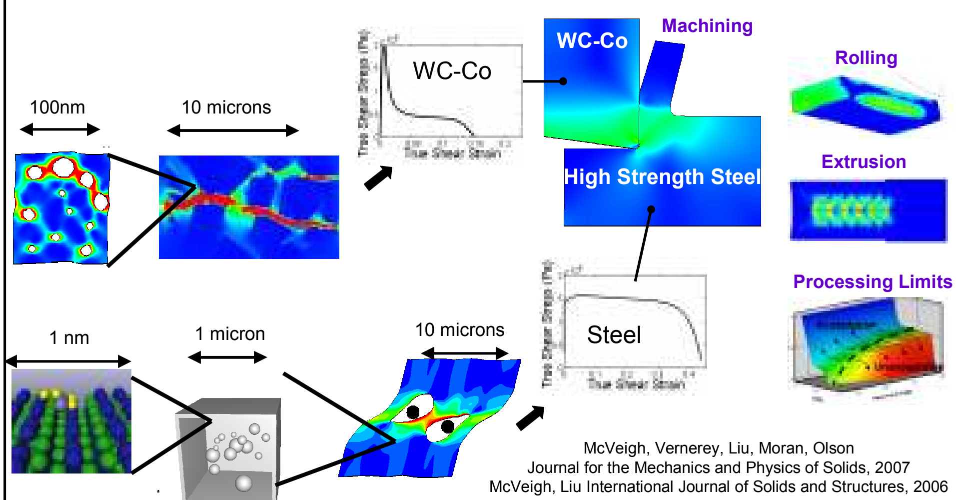
Simulation Based Hierarchical Modeling



Hierarchical Constitutive Modeling

• Hierarchical Modeling of Structure-Property Relations

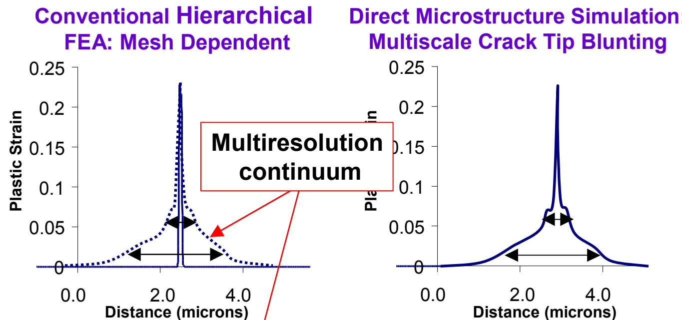
• Macroscale Performance related to microstructural evolution

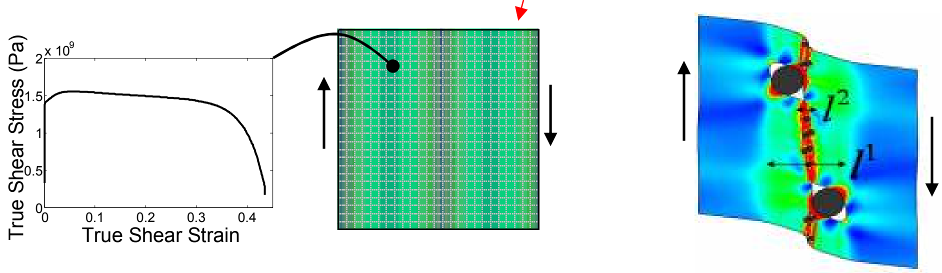


McVeigh, Vernerey, Liu, Moran, Olson
Journal for the Mechanics and Physics of Solids, 2007
McVeigh, Liu International Journal of Solids and Structures, 2006

Capturing the Length Scale of Deformation via Multiresolution Probabilistic Finite Element Method

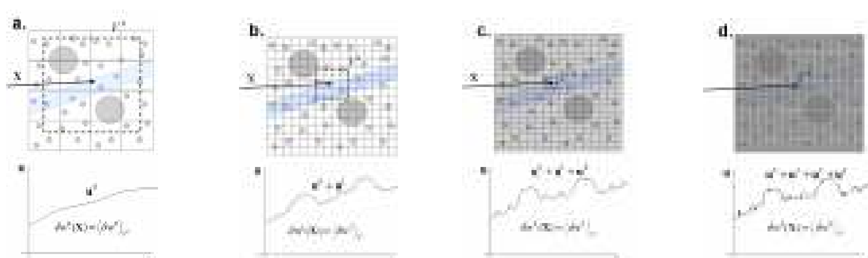
- Conventional Multiscale Methods: cannot handle inhomogeneous deformation
- Extend continuum to inhomogeneous deformation





Multiresolution Imaging vs Microstructure

Increasing Field & Constitutive Resolution



Small Number of degrees of freedom – suitable for average behavior

Discrete behavior of larger particles begins to be observed

Discrete behavior of smaller particles is observed

Very fine resolution – all individual micro-constituents

Small Number of pixels per km^2 – suitable for a global image

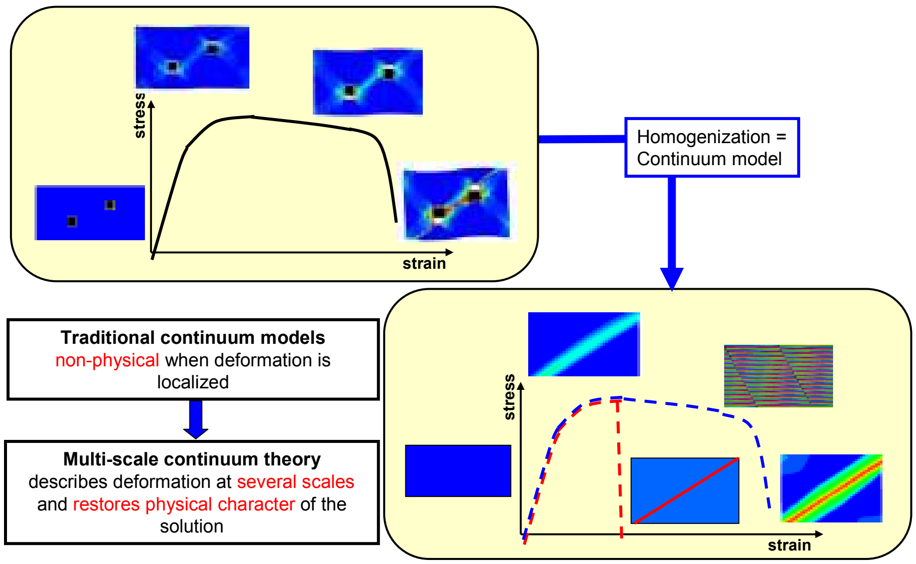
More resolution – cities can be observed

Increasing resolution – buildings can be observed

Northwestern University - a fine institution

Increasing Image Resolution

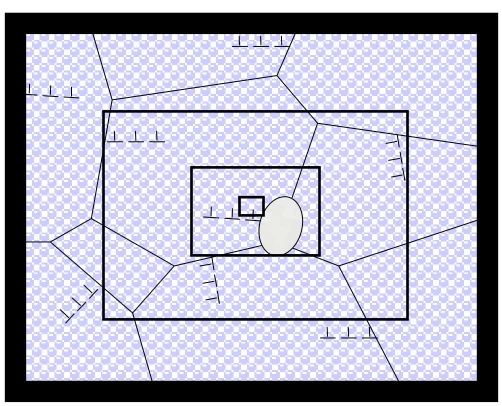
Multi-Scale Continuum Theory



Multiresolution Imaging and Statistical Analysis

• Conventional approach: approximate average macroscale response, continuum mechanics

• Theoretically the average microstructure response can be determined at any scale



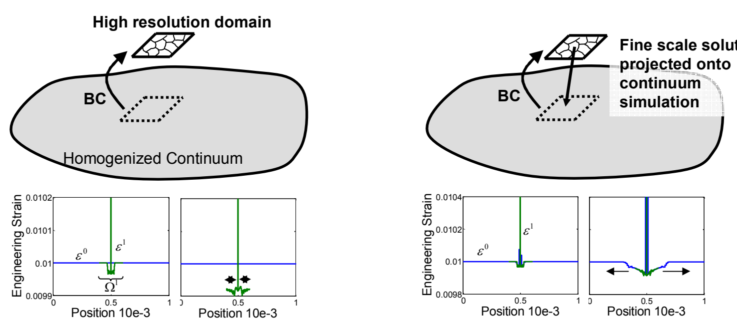
• Practically, we chose the key scale at which deformation and failure is dominant
E.g. macroscale ~m, mesoscale ~ mm, microscale ~microns, sub-microscale ~ nm

Introduction

- Microstructure determines the material’s processing behavior, mechanical and physical properties and product performance.
- Direct numerical simulation (DNS) of the heterogeneous microstructure (dislocations, grain boundaries, interfaces, embedded particles) remains prohibitively expensive due to the vast scale difference between the component and the underlying microstructure.
- Homogenization theory
  - used extensively for modeling the average behavior of the microstructure.
  - fails when a local heterogeneity strongly influences the overall behavior.
- Improvements proposed here
  - To improve upon the conventional continuum homogenization approach where necessary by including extra microscale information either through direct numerical simulation (DNS) of the microstructure over a limited region, or by introducing a microscale non-local behavior through inclusion of the microscale deformation gradient.
- Predictive multiscale, multiresolution theory and multiscale continuum (Liu and McVeigh,. Computational Mechanics, 2007).

The Concurrent and Hierarchical Approaches

Hierarchical Approach **Concurrent Approach**



We begin by decomposing the body into ‘scales’

Each scale is progressively smaller i.e. more fine scale details can be modeled

The deformation is decomposed where the scales overlap

Discussion

- Hierarchical and concurrent theories:
  - Hierarchical approach: simple but only one way information passing, more suited for static problems.
  - Concurrent approach is more accurate for both static and transient problems but has more complicated data structure.
  - Both provide improved resolution by refined mesh;
  - Both are traditional continuum theory-based:
    - For strength and toughness problems they suffer from the problems of conventional continuum approaches (e.g. pathological mesh dependence in softening materials).
- **Gradient Enhanced Multiscale Continua**
  - To include the scale of deformation in governing equation.
  - A power equivalence based formulation (Liu, McVeigh 2007).

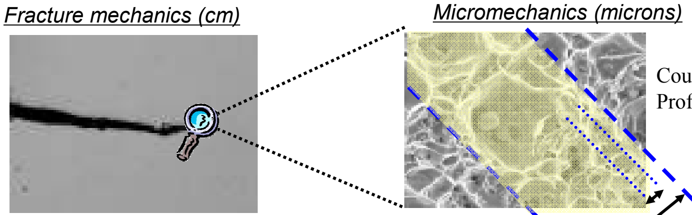
Scope

- We start with materials design subject to thermal mechanical conditions, using strength, hardness and toughness of alloys and cemented composites as examples.
- Use similar multiresolution theories for functional materials design for thermal-mechanical-(radiation enhanced) mass diffusion-electrical efforts.
- The focus is on multiple temporal and spatial scales modeling and simulations.
- Applications to nanoscale sensing, actuation, energy generation functional materials, with focus on durability and reliability with minimum performance lost.

Motivation for Gradient Enhanced Multiscale Continua

- **Mathematical formulation for virtual materials design**

Fracture mechanics (cm) *Micromechanics (microns)*



Courtesy Prof. Olson

- **Current mathematical models**
  - Continuum models based on homogenization theory => No length scale
  - Non-local continuum models. => Only one length scale and empirical
  - Microstructure modeling => Computationally expensive

- **Multi-scale continuum theory**
  - Constitutive relation is determined in terms of microstructure parameters
  - Computationally efficient
  - Describe materials with several length scales

Metal Alloy: Heterogeneous Microstructure

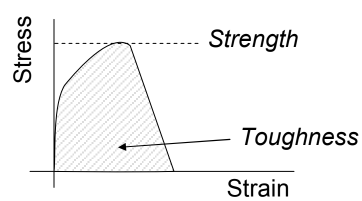
Precipitates created through heat treatments

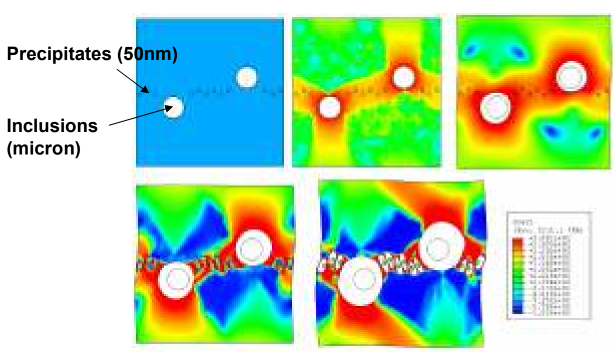
Increase strength by impeding dislocations

Debond to nucleate voids and decrease fracture toughness

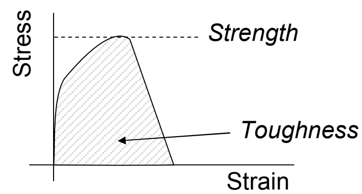
Inclusions are a processing by-product

Nucleate voids causing strain localization and decrease fracture toughness





Metal Alloy: Optimization of Design Variables



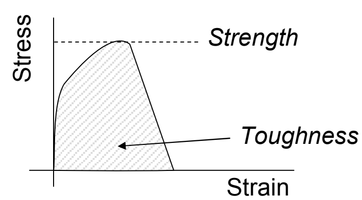
Macroscopic Properties are controlled by many microstructural variables

For computational materials design we choose the key design variables, e.g.:

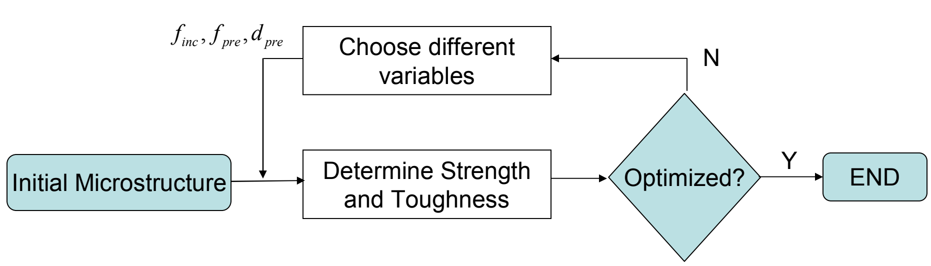
For Strength
• Important variables: precipitate spacing and size

For Toughness
• Important variables: inclusion volume fraction, precipitate volume fraction, debonding behavior

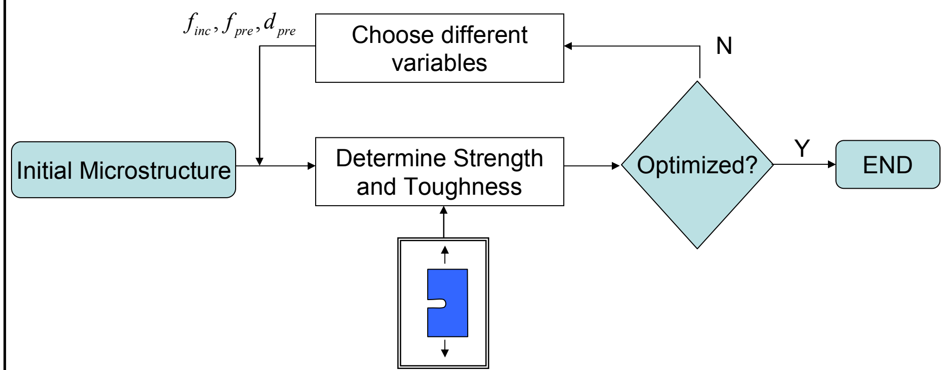
Metal Alloy : Optimization



Optimization and Design



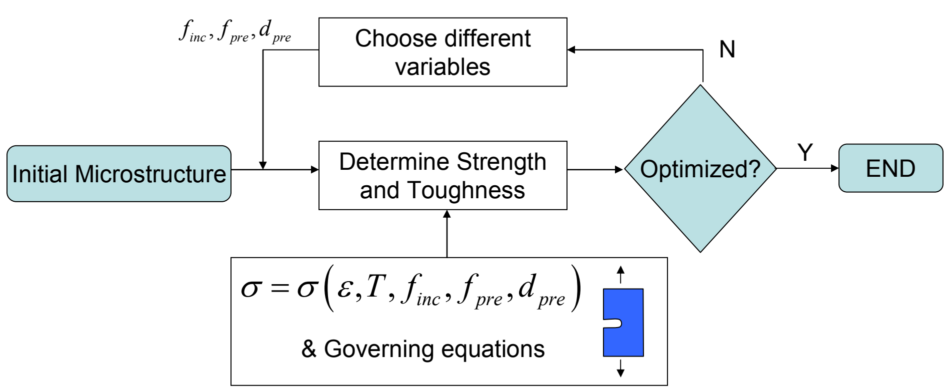
Metal Alloy : Optimization



Determine Strength and Toughness?

- Experimentally – takes years (traditional approach)
- Use a mathematical model of the microstructure
    - Directly model microstructure OR
    - Homogenized material model w/ parameterized microstructure e.g. hierarchical

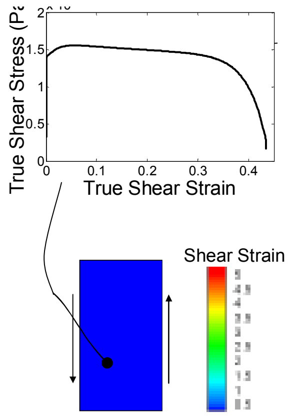
Optimizing a homogenized representation of the microstructure

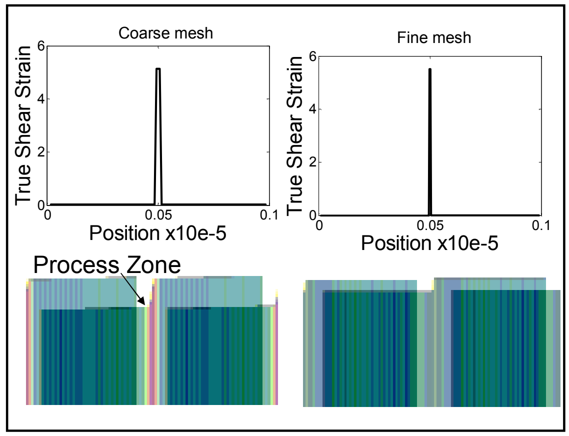


Problems
- Fracture toughness is a function of the softening behavior
- Homogenization cannot handle softening
- Homogenization cannot be used to determine fracture toughness physically

Simulated Localization using Homogenization

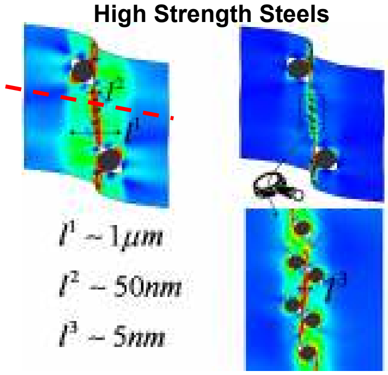
- Localization (process zone) in a single band of elements
- Fracture toughness will be unphysical

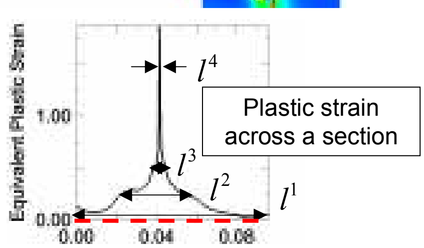




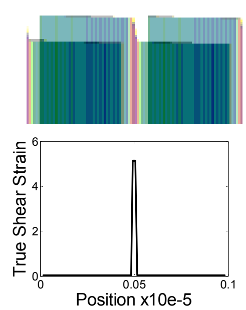
In the real microstructure, localization zone width is related to the microstructure

Localization in a Real Microstructure





1. Localization at the scale of the inclusions
2. Localization at the scale of the precipitates
3. Localization on the shear plane due to microvoid tails



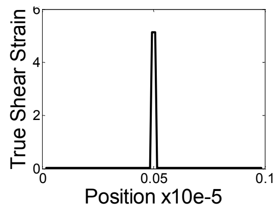
Compare to homogenized solution

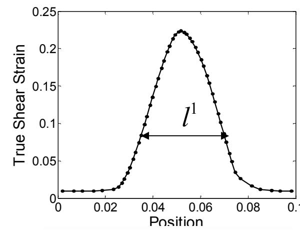
Capturing the localization scale

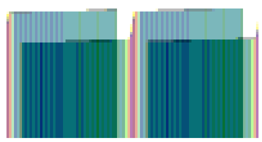
- Strain gradient models
  - Smooth out the localizing strain over a length scale l^1
  - Results are mesh independent

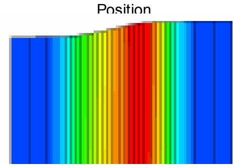
Couple stress Strain Gradient

$$\delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F}^T \qquad \delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F}^T + \mathbf{Q} \vdots \delta\nabla\mathbf{F}^T$$







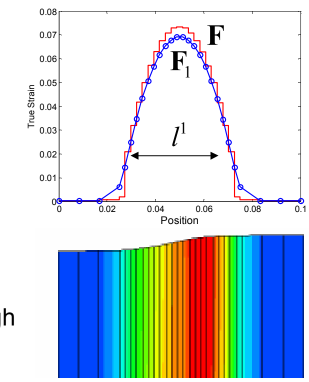


Localization length scale: Gradient Models

- Cannot be formulated as a design problem
  → Difficult to determine material parameters and relations
- Physical interpretation of the couple stress not well understood
- Is limited to regularization over a SINGLE scale only
- Requires higher order shape functions
  → Second gradient of the displacement $\nabla\mathbf{F}^T$
- Proposed Multiscale Gradient Continuum Approach
  - Uses gradients of independent fields to regularize the solution at various scales
  - Each gradient is a physical quantity
  - Each higher order stress represents a distinct microscale behavior
  - Can predict the multiscale nature of localization
  - Can be used to model the process zone physically
  - Returns physical fracture toughness results for materials design

Multiple Localization Scales

$$\delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F}^T + \mathbf{Q} \vdots \delta\nabla\mathbf{F}^T$$



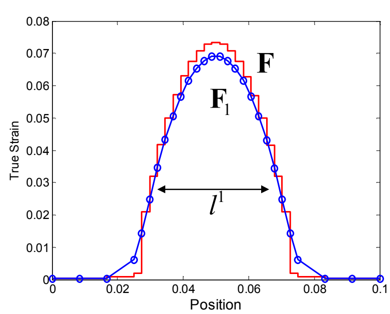
- Consider what happens if we
  - → Introduce a *dummy* strain field
  - → Solve directly for the *dummy* strain field
  - → Constrain the *dummy* strain field to the real deformation using a lagrange multiplier

$$\delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F}^T + \boldsymbol{\beta} : \delta\left(\mathbf{F}_1^T - \mathbf{F}^T\right) + \mathbf{Q} \vdots \delta\nabla\mathbf{F}_1^T$$

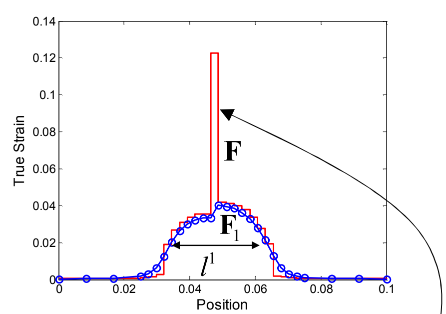
- Expressions are equal if $\boldsymbol{\beta}\left(\mathbf{F}_1^T - \mathbf{F}^T\right)$ is stiff enough
- What happens if the lagrange multiplier is relaxed?

Multiple Localization Scales

$$\delta w^{\text{int}} = \mathbf{P} : \delta\mathbf{F}^T + \boldsymbol{\beta} : \delta\left(\mathbf{F}_1^T - \mathbf{F}^T\right) + \mathbf{Q} \vdots \delta\nabla\mathbf{F}_1^T$$



With constraint



Constraint is relaxed

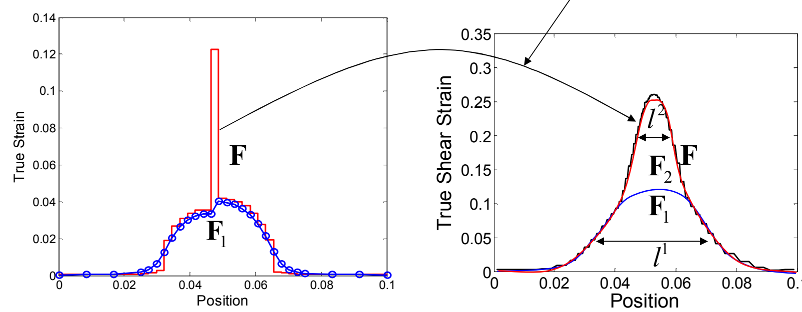
When the constraint is relaxed:
→ The conventional continuum equations are returned
→ Strain localizes again in a single element

Can we control the localizing strain at another smaller scale?

Introducing Further Scales

Constrain the conventional strain to another strain $\mathbf{F}_2$

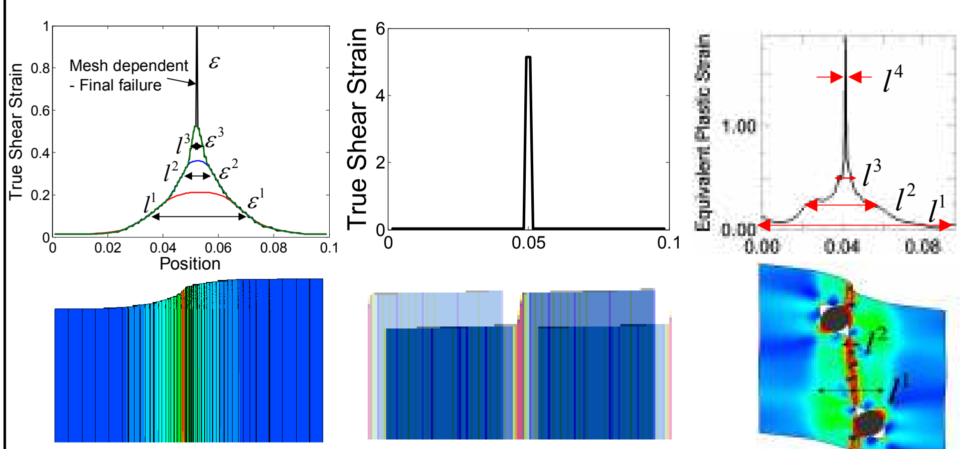
$$\delta w^{\text{int}} = \mathbf{P} : \delta \mathbf{F}^T + \boldsymbol{\beta}_1 : \delta\left(\mathbf{F}_1^T - \mathbf{F}^T\right) + \mathbf{Q}_1 \vdots \delta\nabla\mathbf{F}_1^T + \boldsymbol{\beta}_2 : \delta\left(\mathbf{F}_2^T - \mathbf{F}^T\right) + \mathbf{Q}_2 \vdots \delta\nabla\mathbf{F}_2^T$$



The plastic strain is now regularized at two different scales
The same approach can be generalized to N scales

Multiscale Localization

$$\delta w^{\text{int}} = \mathbf{P} : \delta \mathbf{F}^T + \sum_{n=1}^{N}\left(\boldsymbol{\beta}_n : \delta\left(\mathbf{F}_n^T - \mathbf{F}^T\right) + \mathbf{Q}_n \vdots \delta\nabla\mathbf{F}_n^T\right)$$



Multiscale Continuum
N=3
50 elements

Compare to conventional homogenized solution
25 elements

Compare to microstructure
2500 elements

Proposed Approach: A Multiresolution Continuum Governing Equation

High Strength Steel

• Steel alloy matrix contains precipitates (~50nm) and inclusions (~1micron)

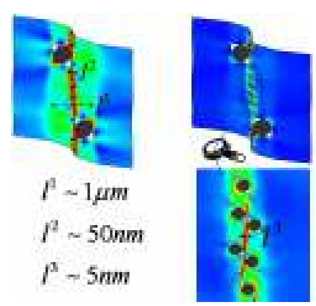
• Weakly bonded inclusions debond nucleating large voids

• Strain localizes between large voids (~micron)

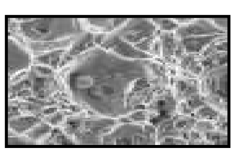
• Precipitates debond in localizing region, nucleating small voids

• Strain localizes between small voids (~50nm)

• Two scales of strain localization



http://www.stress.com/metlab/scope-ductile.htm

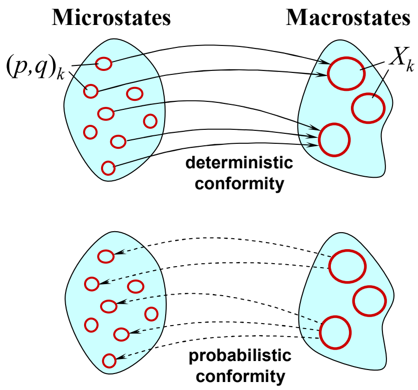


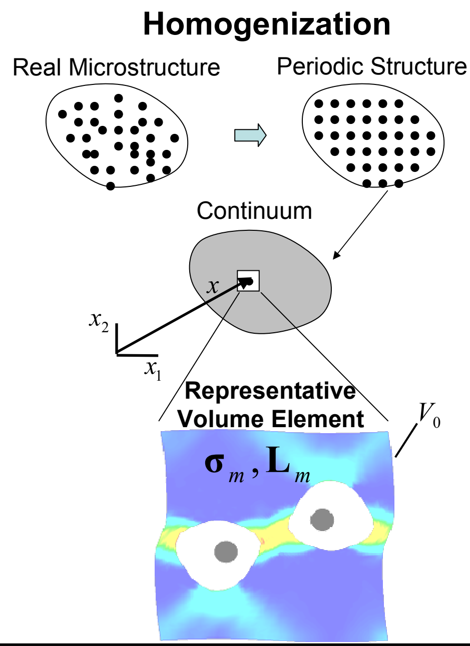
Fracture surface : (primary inclusion voiding and small (secondary) particle voiding)

There are **three clear length scales** involved in ductile failure of high strength steels

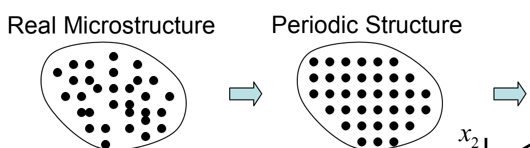
Relation of Statistical Description of Mechanical Systems to Homogenization

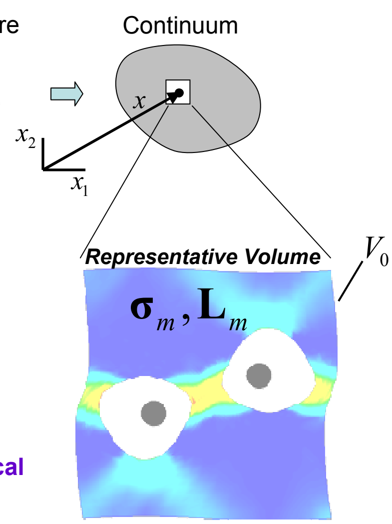
From the contemporary point of view, statistical mechanics can be regarded as a hierarchical *multiscale method*, which eliminates the atomistic degrees of freedom, while establishing a *deterministic* mapping from the atomic to macroscale variables, and a *probabilistic* mapping from the macroscale to the atomic variables:





Classical Homogeneous Deformation Approximation





• Hill condition: relates microstructure to continuum point

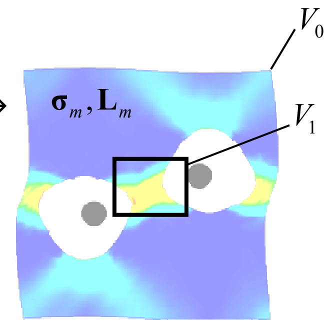
$$
\begin{aligned}
\delta p^{\text{int}} &= \frac{1}{V_0}\int_{V_0} \boldsymbol{\sigma}_m : \delta \mathbf{L}_m^T \, dV_0 \\
&\approx \left(\frac{1}{V_0}\int_{V_0} \boldsymbol{\sigma}_m \, dV_0\right) : \left(\frac{1}{V_0}\int_{V_0} \delta \mathbf{L}_m^T \, dV_0\right) \\
&= \boldsymbol{\sigma} : \delta \mathbf{L}^T \\
&= \delta p_{\text{hom}}^{\text{int}}
\end{aligned}
$$

Macroscale Statistical Averaging

The strain is assumed to vary *homogeneously* over a large range >> V_0

Extension to Inhomogeneous Deformation via Nested Statistical Averaging

- Strain may be strongly inhomogeneous
- E.g. between neighboring voids, localization occurs →



- Extend Hill's condition to account for inhomogeneous deformation

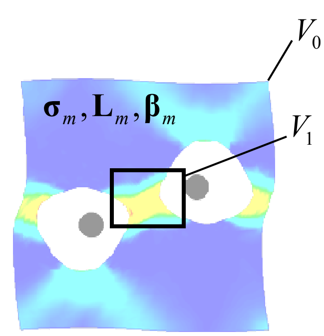
$$\delta p^{\text{int}} = \delta p^{\text{int}}_{\text{hom}} + \delta p^{\text{int}}_{\text{het}}$$
$$= \boldsymbol{\sigma} : \delta \mathbf{L}^T + \frac{1}{V_1}\int_{V_1} \left(\boldsymbol{\sigma}_m : \delta \mathbf{L}_m^T - \boldsymbol{\sigma} : \delta \mathbf{L}^T \right) dV_1$$

Microscale Statistical Averaging

- Statistical averaging performed at two resolutions in internal power expression

Inhomogeneous Power Equivalence

- Rewrite inhomogeneous power in terms of $\delta \mathbf{L}_m - \delta \mathbf{L}$



$$\delta p^{\text{int}} = \boldsymbol{\sigma} : \delta \mathbf{L}^T + \frac{1}{V_1}\int_{V_1} \left(\boldsymbol{\sigma}_m : \delta \mathbf{L}_m^T - \boldsymbol{\sigma} : \delta \mathbf{L}^T \right) dV_1$$

power equivalence

$$\delta p^{\text{int}} = \boldsymbol{\sigma} : \delta \mathbf{L}^T + \frac{1}{V_1}\int_{V_1} \boldsymbol{\beta}_m : \left(\delta \mathbf{L}_m^T - \delta \mathbf{L}^T \right) dV_1$$

- Assume linear variation of $\mathbf{L}_m(y) = \mathbf{L}_m(x) + \nabla \mathbf{L}_m(x)$
- Perform the small scale **statistical averaging operation**

$$\delta p^{\text{int}} = \boldsymbol{\sigma} : \delta \mathbf{L}^T + \boldsymbol{\beta}^1 : (\delta \mathbf{L}^1 - \delta \mathbf{L})^T + \overline{\boldsymbol{\beta}}^1 \vdots \delta \nabla \mathbf{L}^1$$

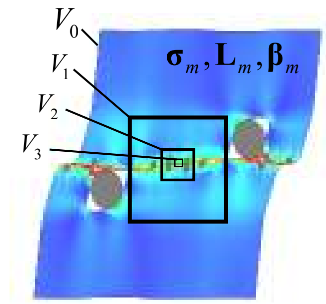
→ a continuum expression

- 'Microstress' represents resistance to inhomogeneous deformation at scale V_1

$$\boxed{\boldsymbol{\beta}^1 = \frac{1}{V_1}\int_{V_1} \boldsymbol{\beta}_m dV_1} \qquad \boxed{\overline{\boldsymbol{\beta}}^1 = \frac{1}{V_1}\int_{V_1} \boldsymbol{\beta}_m \mathbf{y} dV_1}$$

Multiscale Inhomogeneous Deformation

- Many materials exhibit inhomogeneous behavior at several scales



- Simply extend the internal power expression:

$$\delta p^{\text{int}} = \boldsymbol{\sigma} : \delta \mathbf{L}^T + \sum_{n=1}^{N} \boldsymbol{\beta}^n : (\delta \mathbf{L}^n - \delta \mathbf{L})^T + \overline{\boldsymbol{\beta}}^n \,\vdots\, \delta \nabla \mathbf{L}^n$$

- 'Microstress' represents resistance to inhomogeneous deformation at scale V_n

$$\boxed{\boldsymbol{\beta}^n = \frac{1}{V_n} \int_{V_n} \boldsymbol{\beta}_m \, dV_n} \qquad \boxed{\overline{\boldsymbol{\beta}}^n = \frac{1}{V_n} \int_{V_n} \boldsymbol{\beta}_m \mathbf{y} \, dV_n}$$

All stresses in terms of known microstructural quantities $\boldsymbol{\sigma}_m, \mathbf{L}_m$ only

Multiresolution Continuum

Continuum theory can be extended to capture multiscale physics through the continuum virtual power expressions

Extra *inhomogeneous* contributions to virtual power

$$\delta P_{int} = \int_\Omega \left(\boldsymbol{\sigma} : \delta \mathbf{D} + \sum_{I=1}^{N-1} \left\{ \overline{\boldsymbol{\beta}}^I : (\delta \mathbf{L}^I - \delta \mathbf{L}) + \overline{\overline{\boldsymbol{\beta}}}^I \,\vdots\, \delta \mathbf{L}^I \overleftarrow{\nabla} \right\} \right) d\Omega$$

$$\delta P_{ext} = \int_\Omega \mathbf{b} \cdot \delta \mathbf{v} \, d\Omega + \int_{\Gamma_t} \mathbf{t} \cdot \delta \mathbf{v} \, d\Gamma + \int_\Omega \sum_{I=1}^{N-1} \mathbf{B}^I : \delta \mathbf{L}^I d\Omega + \int_{\Gamma_t} \sum_{I=1}^{N-1} \mathbf{T}^I : \delta \mathbf{L}^I d\Gamma$$

$$\delta P_{kin} = \int_\Omega \left\{ \rho \dot{\mathbf{v}} \cdot \delta \mathbf{v} + \sum_{I=1}^{N-1} \left(\boldsymbol{\gamma}^I \cdot \mathbf{I}^I \right) : \delta \mathbf{L}^I \right\} d\Omega$$

Conventional Continuum Expressions **Extension to Multiscale**

Multiresolution Governing Equations

$$\boldsymbol{\sigma} - \sum_{n=1}^{N} \boldsymbol{\beta}^{nT} + \mathbf{b} = 0 \quad \text{in} \quad \Omega$$

$$\nabla \cdot \bar{\boldsymbol{\beta}}^{n} - \boldsymbol{\beta}^{n} + \mathbf{B}^{n} = 0 \quad \text{in} \quad \Omega$$

$$\mathbf{t} = \mathbf{N} \cdot \left(\boldsymbol{\sigma} - \sum_{n=1}^{N} \boldsymbol{\beta}^{nT} \right) \quad \text{on} \quad S$$

$$\mathbf{R}^{n} = \mathbf{r}^{n}\mathbf{N} = \mathbf{N} \cdot \bar{\boldsymbol{\beta}}^{n} : (\mathbf{NN}) \quad \text{on} \quad S$$

$$\left\| \mathbf{N} \cdot \left(\boldsymbol{\sigma} - \sum_{n=1}^{N} \boldsymbol{\beta}^{nT} \right) \right\| = 0 \quad \text{on} \quad \Gamma$$

$$\left\| \mathbf{N} \cdot \bar{\boldsymbol{\beta}}^{n} \right\| = 0 \quad \text{on} \quad \Gamma$$

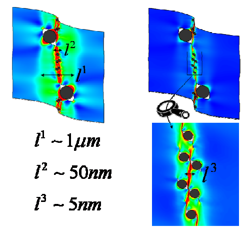
Constitutive Relationships $\dot{\boldsymbol{\sigma}}(\mathbf{L}), \dot{\boldsymbol{\beta}}^{n}(\mathbf{L}^{n} - \mathbf{L}), \dot{\bar{\boldsymbol{\beta}}}^{n}(\mathbf{G}^{n})$

Proposed Approach: Multiresolution Continuum Constitutive Equations

Multiscale Localization

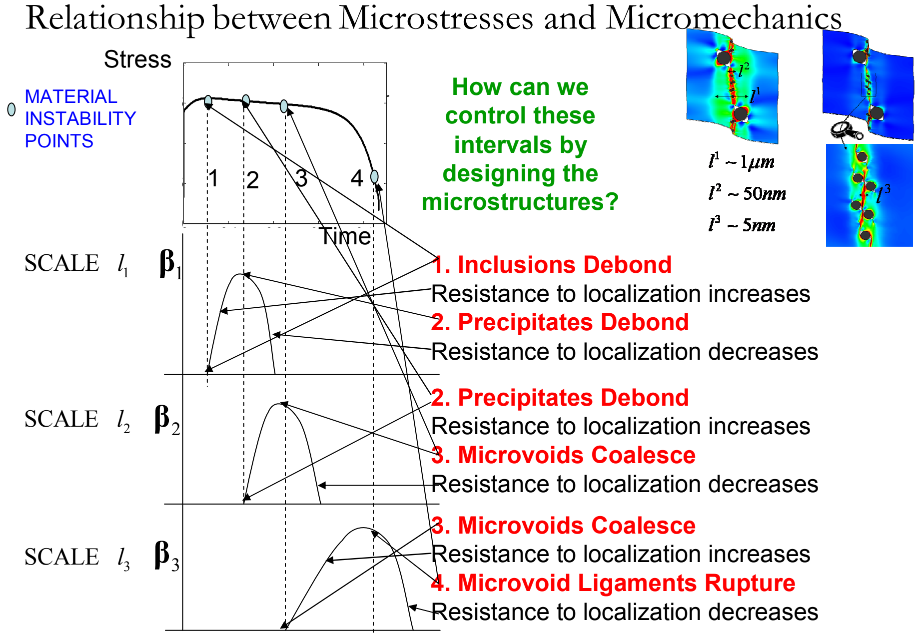
$$\delta w^{\text{int}} = \mathbf{P} : \delta \mathbf{F}^T + \sum_{n=1}^{N} \left(\boldsymbol{\beta}_n : \delta\left(\mathbf{F}_n^T - \mathbf{F}^T\right) + \mathbf{Q}_n \vdots \delta \nabla \mathbf{F}_n^T \right)$$

- The Lagrange Multiplier has a physical meaning – it is a Microstress
- Represents resistance to localization
- This resistance is controlled by microstructural events in alloys
- When the inclusions debond, localization occurs at l_1
- When the precipitates debond, localization occurs at l_2
- When the voids grow and coalesce in the shear plane, localization occurs at l_3



- These events correspond to microstress instability points which are captured in the macroscale stress-strain relation

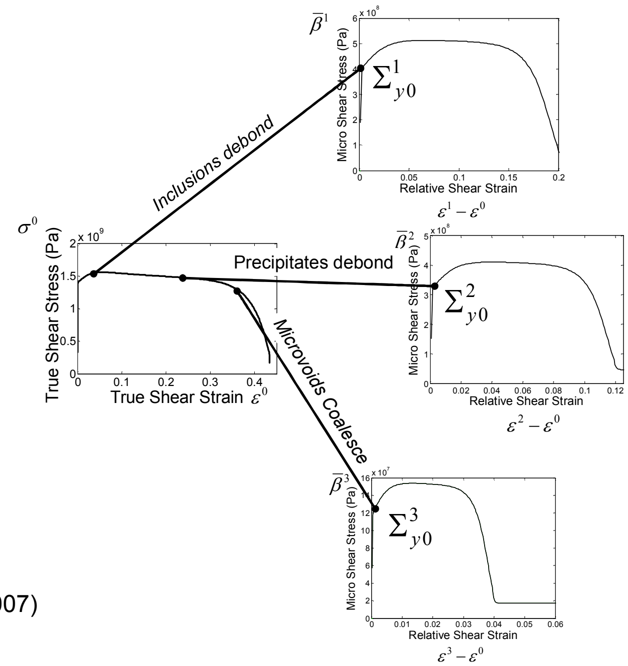
Relationship between Microstresses and Micromechanics



Multiscale Constitutive Behavior is derived from a Power Equivalence Approach

Constitutive relationships computed at each scale using a statistical cell modeling procedure.

The constitutive behavior is closely related to the key microscale events.



Liu and McVeigh, 2007)

Summary: Traditional FE versus Multiresolution FE

Equilibrium Equations	
$\nabla\square\boldsymbol{\sigma} + \mathbf{b} = 0 \quad \text{in} \quad \Omega$ $\mathbf{N}\square\boldsymbol{\sigma} - \mathbf{t} = 0 \quad \text{on} \quad S$	$\nabla\square\left(\boldsymbol{\sigma} - \sum_{n=1}^{N}\boldsymbol{\beta}^{nT}\right) + \mathbf{b} = 0 \quad \text{in} \quad \Omega$ $\nabla\square\bar{\boldsymbol{\beta}}^n - \boldsymbol{\beta}^n + \mathbf{B}^n = 0 \quad \text{in} \quad \Omega$ $\mathbf{N}\square\left(\boldsymbol{\sigma} - \sum_{n=1}^{N}\boldsymbol{\beta}^{nT}\right) - \mathbf{t} = 0 \quad \text{on} \quad S$
Stress and strain	
Stress : $\boldsymbol{\sigma}$ Strain : $\mathbf{L}$	Stress : $\boldsymbol{\Sigma} = \left[\boldsymbol{\sigma} \quad \boldsymbol{\beta}^1 \quad \bar{\boldsymbol{\beta}}^1 \quad \cdots \quad \boldsymbol{\beta}^N \quad \bar{\boldsymbol{\beta}}^N\right]$ Strain : $\boldsymbol{\Delta} = \left[\mathbf{L} \quad \left(\mathbf{L}^1 - \mathbf{L}\right) \quad \mathbf{L}^1\overleftarrow{\nabla} \quad \cdots \quad \left(\mathbf{L}^N - \mathbf{L}\right) \quad \mathbf{L}^N\overleftarrow{\nabla}\right]$
Internal power	
$p_{\text{int}} = \boldsymbol{\sigma} : \mathbf{L}$	$p_{\text{int}} = \boldsymbol{\Sigma} \cdot \boldsymbol{\Delta}$
Constitutive Relationships	
$\boldsymbol{\sigma}^{\nabla} = \mathbf{C}^{ep} : \mathbf{L}$	$\boldsymbol{\Sigma}^{\nabla} = \square^{ep} : \boldsymbol{\Delta}$