Composite Properties and Microstructure II: Strength

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Composites: Where Mathematics Meets Industry

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Structure and substructure - form and functionality - across multiple length scales

Racing Sail

Fiber reinforced epoxy
Horizontal Stabilizer
Boeing 777

Bone
Multi-scale problem statement

It is supposed that the length scale of the composite microstructure is significantly smaller than the length scale of the load.

To characterize failure initiation inside the composite it is required to assess the extreme field behavior at the length scale of the microstructure generated by macroscopic loading.
Microstructures considered in this presentation: Graded Locally Periodic Microstructure

Length scales:
Microstructure length scale relative to load length scale is denoted by $\varepsilon$
Consider also the random two phase layered composite

Partition the plane into strips of unit width. Over strip each flip a coin: if heads strip is black if tails strip is white.

Probability of heads is $\theta$
Probability of tails is: $1 - \theta$
Random laminar microstructure inside L-shaped domain

For a given realization of the Layered random medium rescale it by 1/40 and inlay it inside the L-shaped domain
Study two complementary aspects of stress transfer

- Assess extent of overstressed zones in composite structures due to reentrant corners, bolt holes, rivets and other stress risers
- Lower bounds on maximum local fields inside random microstructure due to macroscopic loading
The first part of this talk outlines a mathematically rigorous methodology for bounding overstressed zones inside composite materials due to stress risers.
Boundary value problem in microstructured elastic media

Length scale of microstructure \( 0 < \varepsilon << 1 \)

Elastic displacement field \( u^\varepsilon(x) \)
Strain tensor \( \varepsilon^\varepsilon(x) \)
\( \varepsilon^\varepsilon = \frac{1}{2}(u^\varepsilon_{i,j} + u^\varepsilon_{j,i}) \)

Stress tensor \( \sigma^\varepsilon(x) \)

Local elastic tensor \( C^\varepsilon(x) = C^i \)

\( C^i \) is the elasticity of \( i \)th material

Constitutive relation \( \sigma^\varepsilon(x) = C^\varepsilon(x)\varepsilon^\varepsilon(x) \)

Equation of elastic equilibrium \( -div(\sigma^\varepsilon) = f \)

Boundary conditions:

Traction BC on \( \Gamma_N \)
\( n \cdot \sigma^\varepsilon(x) = g \)

and displacement BC on \( \Gamma_D \)
\( u^\varepsilon = U \)
Homogenization theory; convergence of averages

For any subset $S$:

\[
\int_{S} u^{\varepsilon} (x) dx \rightarrow \int_{S} u^{M} (x) dx
\]
\[
\int_{S} \varepsilon^{\varepsilon} (x) dx \rightarrow \int_{S} \varepsilon^{M} (x) dx \quad \varepsilon^{M} = \frac{u_{i,j}^{M} + u_{j,i}^{M}}{2}
\]
\[
\int_{S} \sigma^{\varepsilon} (x) dx \rightarrow \int_{S} \sigma^{M} (x) dx
\]

Homogenized constitutive relation

\[
\sigma^{M} (x) = C^{E} (x) \varepsilon^{M} (x)
\]
\[
- \text{div} \sigma^{M} = f
\]
\[
\mathbf{u}^{M} = U
\]
\[
n \cdot \sigma^{M} (x) = g
\]
Formula for $C^E$

- Load unit RVE with homogeneous strain $\bar{\varepsilon}$
- Local elastic tensor in microstructure $= C(y)$
- Micro-problem in RVE for local strain fluctuation
- Local strain fluctuation $e(y)$ solves:
  \[
  \text{div} \left( C(y)(e(y) + \bar{\varepsilon}) \right) = 0
  \]
- $C^E$ given by:
  \[
  C^E \bar{\varepsilon} = \int_Q C(y)(e(y) + \bar{\varepsilon}) dy
  \]
Stress Bound Part 1

Stress in composite = $\sigma^\varepsilon, 0 < \varepsilon \ll 1$

Stress in i-th phase = $\sigma_i^\varepsilon(x)$

Set of interest ``S''

Consider quadratic invariants of the stress tensor, e.g., Von Mises stress, square of dilatational stress. These are written as: $\prod (\sigma_i^\varepsilon(x))$

Stress bound on S: For almost every x in S and for $\varepsilon$ sufficiently small,

$$\prod (\sigma_i^\varepsilon(x)) \leq \sup_{x \in S} f^{(i)}(x, \text{microgeometry})$$

Computation of Stress Bound – Multi Scale Analysis: Step 1 - Up scaling

- Replace local elastic properties with effective elastic property $C^E(x)$.
- Find homogenized stress $\sigma^M(x)$
- Find homogenized strain $\varepsilon^M(x)$

\[
\sigma^M(x) = C^E(x)\varepsilon^M(x)
\]

\[-\text{div} \sigma^M = f\]
Step 2. Down scaling

- Load unit RVE with homogenized strain $\varepsilon^M(x)$
- Local elastic tensor in microstructure = $C(y)$
- Micro-problem in RVE for local strain fluctuation
- Local strain fluctuation $e(x,y)$ solves:
  
  \[
  \text{div} \left( C(y)(e(x,y) + \varepsilon^M(x)) \right) = 0
  \]

- Strain fluctuation in i-th phase: $e_i(x,y)$
- Stress bound given by:
  
  \[
  f^{(i)}(x, \text{microgeometry}) = \sup_y \prod (C^i(y)(e_i(x,y) + \varepsilon^M(x)))
  \]
Stress Bound Part 2

Over stressed region in i-th phase = \{ x \in V, \text{where}, \prod (\sigma_i^{\varepsilon}(x)) > t \}

Volume of over stressed region in i-th phase = \lambda_i^{\varepsilon}(t)

\left| \left\{ f^{(i)}(x) \geq t \right\} \right| = \text{Volume of set where } f^{(i)}(x) \geq t

Stress bound: \lim_{\varepsilon \to 0} \lambda_i^{\varepsilon}(t) \leq \left| \left\{ f^{(i)}(x) \geq t \right\} \right|

Stress assessment in shaft with L shaped cross section filled with random laminate and subjected to torsion load

$\beta =$ shear compliance in phase 1
$\alpha =$ shear compliance in phase 2
$\alpha < \beta$

$\theta =$ probability of phase 2

Homogenized in-plane stress $\sigma^M = (\sigma_1^M, \sigma_2^M)$

$$\gamma_\alpha = \theta (\beta - \alpha) / (\alpha + (1 - \theta)(\beta - \alpha))$$

$$\gamma_\beta = -(1 - \theta)(\beta - \alpha) / (\alpha + (1 - \theta)(\beta - \alpha))$$

$$f^{(1)}(x) = (1 + \gamma_\alpha)^2 | \sigma_2^M (x) |^2 + | \sigma_1^M (x) |^2$$

$$f^{(2)}(x) = (1 + \gamma_\beta)^2 | \sigma_2^M (x) |^2 + | \sigma_1^M (x) |^2$$
Direct comparison between the homogenized stress and rigorous bounds on overstressed zones inside each elastic material

Up scaling only:
Homogenized stress: $\sigma^M$
Level line of $|\sigma^M|^2$

Up scaling + Down scaling
Gives stress bound and
Encodes effects of stress fluctuation at the level of the microgeometry

Here: $\alpha=2$, $\beta=10$, $\theta=.33$
Optimization of graded microstructure: fiber reinforced shaft subject to torsion

Cylindrical shaft with X-shaped cross section subject to torsion loading. Reinforce with locally layered material. Here relative layer thicknesses can change as well as layer orientation.
Solution of design Problem via inverse homogenization.

Use the effective stiffness and stress bound to identify a locally layered microstructure with the desired properties.

Goal: Design for maximum torsional rigidity while minimizing the effect of the stress concentrations at the reentrant corners.

- Effective stiffness is explicit function of local layer orientation and material 1 area fraction.
- Stress bound explicit function of local layer orientation and material 1 area fraction
- So design variables are local layer orientation and area fraction of material 1

Formulation of design problem

$$\min_{\text{Designs}} \{-\text{Rigidity} + \lambda \iint (f^{(i)})^p dx_1 dx_2\}$$

$$\beta = 0.5 \quad \text{- Compliance in shear for compliant material}$$

$$\alpha = 0.25 \quad \text{- Compliance in shear for stiff material}$$

$$\theta = \text{local area fraction of compliant material} \quad p = 1, 2$$

Resource constraint:

$$\iint (1 - \theta) dx_1 dx_2 \leq C$$
Design 1. Density distribution of compliant material for a shaft optimized for rigidity only

Area of stiff material = 60%
Rigidity = 0.82
Design 2. Density distribution of compliant material for shaft optimized for rigidity subject to constraint on $f^1$

Area of stiff material = 60%  
Rigidity = 0.61
Design 3. Density distribution of compliant material for a shaft optimized for rigidity subject to constraint on $f^2$

Area of stiff material = 60%

Rigidity = 0.62
Contour plots for $f^1$ Designs 1 and 2

Design 1

Design 2
Contour plots for $f^2$ Designs 1 and 3
Consider a sample of composite subjected to a uniform thermal gradient.

In this part of the talk we develop lower bounds for the maximum Temperature gradient generated at the level of the microgeometry.
A realization of a random medium
One and two point correlation functions

One point correlation

Probability of a point lying inside the green phase (Volume fraction of the green phase)

Two point correlation

Probability that both ends of a segment lies in green phase when thrown into composite randomly
One and Two-point Correlation Functions

These statistical functions can be computed using techniques from image analysis. Berryman 1988.
Objectives

Consider the ensemble of composite samples characterized by the same one and two point correlations.

Subject each sample to the same imposed temperature gradient.

Find a lower bound on the maximum temperature gradient inside the samples that is given in terms of the one and two point statistics.

Identify a realization that has the smallest maximum temperature gradient.
Setting

Cube filled with composite made from two heat conductors. The volume fractions of each is prescribed.

Conductivities: \( \sigma_1 > \sigma_2 \)

Volume fractions: \( \theta_1, \theta_2 \)

\[ \Delta T = 0 \quad \text{Inside each phase} \]

\[ n \cdot \sigma_1 \nabla T = n \cdot \sigma_2 \nabla T \quad \text{On interface} \]

\[ \langle \nabla T \rangle = E \quad \text{and} \quad T - E \cdot x \quad \text{is periodic on the cube} \]
First Moment – Effective Properties

$Q_1 = \text{part of cube occupied by phase one}$
$Q_2 = \text{part of cube occupied by phase two}$

Cube domain $= Q = Q_1 \cup Q_2$

$\chi_1 = 1, \text{ in } Q_1, \text{ zero outside}$

$\chi_2 = 1, \text{ in } Q_2, \text{ zero outside}$

$\sigma(x) = \chi_1 \sigma_1 + \chi_2 \sigma_2$

$$\sum^e E = \langle \sigma(x) \nabla T(x) \rangle$$
Earlier work bounds of Hashin and Shtrikman for effective properties

Hashin Shtrikman bounds on effective conductivity for isotropic composites (1962).

\[ \sigma_2 + \frac{3\theta_1 \sigma_2 (\sigma_1 - \sigma_2)}{3\sigma_2 + \theta_2 (\sigma_1 - \sigma_2)} \leq \Sigma^e \]

\[ \Sigma^e \leq \sigma_1 + \frac{3\theta_2 \sigma_1 (\sigma_2 - \sigma_1)}{3\sigma_1 + \theta_1 (\sigma_2 - \sigma_1)} \]
Higher order moments of temperature gradient

Higher moments sensitive to high local thermal gradients

Damage initiation due to high local thermal gradients

\[ \left\langle \chi_1 \mid \nabla T \right\rangle^1/r \quad \infty \geq r \geq 2 \]

\[ \left\langle \chi_2 \mid \nabla T \right\rangle^1/r \quad \infty \geq r \geq 2 \]
Maximum temperature gradients

\[
\lim_{r \to \infty} \langle \chi_1 | \nabla T |^r \rangle^{1/r} = \max_{x \in Q_1} \{ | \nabla T(x) | \}
\]

\[
\lim_{r \to \infty} \langle \chi_2 | \nabla T |^r \rangle^{1/r} = \max_{x \in Q_2} \{ | \nabla T(x) | \}
\]

\[
\| \nabla T \|_{L^\infty(Q)} = \max_{x \in Q} \{ | \nabla T(x) | \}
\]
Optimal Lower Bounds
Isotropic Case I

Hypothesis: isotropic effective thermal properties

For $\infty \geq r \geq 2$

$$\left\langle \chi_1 \mid \nabla T \right|_r^{1/r} \geq \theta_1^{1/r} \frac{\sigma_2}{\sigma_2 + (\sigma_1 - \sigma_2)\theta_2 / 3} \mid E \right|$$

The lower bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material one and coating of material two.

(Lipton J.Appl.Phys.2004(96) 2821-2827)
Optimal Lower Bounds
Isotropic Case II

For $\infty \geq r \geq 2$

$$\left\langle \chi_2 \mid \nabla T \mid r \right\rangle^{1/r} \geq \theta_2^{1/r} \frac{\sigma_1}{\sigma_1 + (\sigma_2 - \sigma_1)\theta_1 / 3} |E|$$

The lower bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material two and coating of material one.

(Lipton J.Appl.Phys.2004(96) 2821-2827)
Optimal Lower Bounds
Isotropic Case III

\[ \| \nabla T \|_{L^\infty(Q)} \geq \frac{\sigma_1}{\sigma_1 + (\sigma_2 - \sigma_1)\theta_1 / 3} |E| \]

The lower bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material two and coating of material one.

(Lipton, J.Appl.Phys.2004(96) 2821-2827)
Anisotropic Mixtures
and the Tensor of Geometric Parameters

Two point correlation function of material one $S_1(r)$

Matrix of geometric parameters "M", J.R. Willis 1977

$M$ is a symmetric matrix and $\text{Trace}\{M\}=1$

$$M = \frac{1}{\theta_1 \theta_2} \sum_{k \neq 0} \hat{S}_1(k) \frac{k \otimes k}{|k|^2}$$

Eigenvalues of $M$: $0 \leq d_1 \leq d_2 \leq d_3 \leq 1$

and $d_1 + d_2 + d_3 = 1$
For $\infty \geq r \geq 2$

$\theta_1$ and $d_1, d_2, d_3$ and $E$ are fixed

$$\left\langle \chi_1 \mid \nabla T \mid^r \right\rangle^{1/r} \geq \theta_1^{1/r} \frac{\sigma_2}{\sigma_2 + (\sigma_1 - \sigma_2)\theta_2 d_3} \mid E \mid$$

The lower bound is attained by the coated ellipsoid assemblage with core of material one and coating of material two with major axis aligned with the imposed temperature gradient $E$.

(Lipton J. Appl. Phys. 2004(96) 2821-2827)
Optimal Lower Bounds
Anisotropic Case II

For $\infty \geq r \geq 2$

$\theta_2$ and $d_1, d_2, d_3$ and $E$ are fixed

$$\left\langle \chi_2 \mid \nabla T \right\rangle^{1/r} \geq \theta_2^{1/r} \frac{\sigma_1}{\sigma_1 + (\sigma_2 - \sigma_1)\theta_1 d_1} \mid E \mid$$

The lower bound is attained by the coated ellipsoid assemblage with core of material two and coating of material one with minor axis aligned with the imposed temperature gradient $E$.

(Lipton J. Appl. Phys. 2004(96) 2821-2827)
Optimal Lower Bounds
Anisotropic Case III

\[ \theta_2 \text{ and } d_1, d_2, d_3 \text{ and } E \text{ are fixed} \]

\[ \| \nabla T \|_{L^\infty(Q)} \geq \frac{\sigma_1}{\sigma_1 + (\sigma_2 - \sigma_1) \theta_1 d_1} \| E \| \]

The lower bound is attained by the coated ellipsoid assemblage with core of material two and coating of material one with minor axis aligned with the imposed temperature gradient \( E \).

(Lipton J. Appl. Phys. 2004(96) 2821-2827)