Composite Properties and Microstructure I: Effective Properties

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Composites: Where Mathematics Meets Industry

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Composite structures

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. The goal is to characterize the behavior of the composite structure when the characteristic length scale of the loading is much larger than the composite microstructure.
Effective properties such as:

1) Effective stiffness
2) Effective thermal conductivity
3) Effective dielectric constant

Are introduced within the context of homogenization theory.
Homogenization theory provides a way to calculate average strain measured by a strain gauge in microstructured media.

- Strain gauge
- Set covered by strain gauge is $S$
- Strain gauge measures average strain over $S$

$\varepsilon = \text{Length scale of microstructure relative to characteristic dimension of loading}$
Boundary value problem in periodically microstructured elastic media

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

Elastic displacement field \( u^\varepsilon(x) \)

Strain tensor \( \varepsilon^\varepsilon(x) = \frac{1}{2}(u_{i,j} + u_{j,i}) \)

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

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

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

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

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

Boundary conditions:

Traction BC on \( \Gamma_N \)

and displacement BC on \( \Gamma_D \)

\( n \cdot \sigma^\varepsilon(x) = g \)

\( u^\varepsilon = U \)
Homogenization theory; convergence of averages

For any subset $S$:
\[
\frac{1}{|S|} \int_S \varepsilon^e(x) dx \to \frac{1}{|S|} \int_S \varepsilon^M(x) dx
\]

Average strain over $S$:
\[
\frac{1}{|S|} \int_S \varepsilon^e(x) dx \to \frac{1}{|S|} \int_S \varepsilon^M(x) dx = \text{Average of homogenized strain}
\]

\[
\frac{1}{|S|} \int_S \sigma^e(x) dx \to \frac{1}{|S|} \int_S \sigma^M(x) dx
\]

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

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

- Load unit RVE with homogeneous strain $\bar{\epsilon}$
- Local elastic tensor in microstructure = $C(y)$
- Micro-problem in RVE is to solve for periodic strain fluctuation
- Local periodic strain fluctuation $e(y)$ solution of:

$$\text{div} \left( C(y)(e(y) + \bar{\epsilon}) \right) = 0, \quad \int_{Q} e(y) \, dy = 0$$

- $C^E$ given by:

$$C^E \bar{\epsilon} = \int_{Q} C(y)(e(y) + \bar{\epsilon}) \, dy$$

Here: $Q$ denotes the RVE
Physical interpretation of the effective elastic tensor $C^E$

Local stress inside RVE

$$\sigma(y) = (C(y)(e(y) + \bar{\varepsilon}))$$

Average strain over RVE

$$\int_Q (e(y) + \bar{\varepsilon}) \, dy = \bar{\varepsilon}$$

Effective elasticity relates average stress to average strain

$$\int_Q \sigma(y) \, dy = C^E \bar{\varepsilon}$$
Approximate formulas for effective elastic tensors

Given only a partial statistical description of the microstructure the goal is to construct an approximation to the effective tensor

Two well known examples are considered

1) Low volume fraction expansions for dilute suspensions. J.C Maxwell (1873), A. Einstein (1906)
2) Low contrast expansions. W.F. Brown (1955)
Effective elastic tensor for a dilute suspension of spheroids

Data:

- $C_1 =$ elastic modulus of spheroids
- $C_2 =$ elastic modulus of matrix,
- $\theta =$ volume fraction of spheroids
Expand $C^E$ in a Taylor series with respect to volume fraction

$$C^E = C_2 + \sum_{j=1}^{\infty} B_j \theta^j$$

The coefficients $B_j$ encode geometry of the distribution of the particles in the suspension, eg., they reflect clumping together of the particles, etc.

$B_1$ is associated with the single particle boundary value problem in an infinite matrix subject to applied field averaged over all orientations

$B_2$ associated with a two particle boundary value problem in infinite matrix averaged over all two particle configurations

$B_j$ associated with $j$ particle boundary value problem in infinite matrix.
The expansion when only the volume fraction and orientation distribution is known

\[ C^E = C_2 + B_1 \theta + O(\theta^2) \]

\[ B_1 = \langle (C_1 - C_2) T_1 \rangle \]

Here brackets denote orientation average and \( T_1 \) is the Wu strain tensor
and \( E \) is the spheroid domain.

The fluctuating part of the strain solves a boundary value problem on the whole space:

\[ \mathbf{T}_1 \bar{\varepsilon} = \frac{1}{|E|} \int_E (e^\infty(y) + \bar{\varepsilon}) dy \]

\[ \text{div}(C(y)(e^\infty(y) + \bar{\varepsilon})) = 0 \]

\[ \lim_{R \to \infty} \frac{1}{|B(R)|} \int_{B(R)} |e^\infty(y)|^2 \, dy = 0 \]

\( B(R) \) is a Ball of radius \( R \) and
Low volume expansion for spheres

$C_1$ isotropic and specified by $\mu_1/\kappa_1$
$C_2$ isotropic and specified by $\mu_2/\kappa_2$
Material 1 incompressible: $\mu_1/\kappa_1 = 0$
Material 2 incompressible: $\mu_2/\kappa_2 = 0$

Low volume expansion for the effective shear modulus

$$\mu^E = \mu_2 + \frac{5(\mu_1 - \mu_2)}{2\mu_1 + 3\mu_2} \theta + O(\theta^2)$$

Established rigorously using variational methods by J.B. Keller, L. Rubenfeld, and J. Molyneux (1967)

For rigid spheres $\mu_1/\mu_2 = \infty$ have Einstein’s formula (1906)

$$\mu^E = \mu_2 + \frac{5}{2} \theta + O(\theta^2)$$
Formulas for higher order terms in expansion of elastic tensor see, Chen and Acrivos (1978)

For complete references and detailed derivations we refer to the recent manuscripts of G. Milton (2002) and S. Torquato (2002)
Low contrast expansions

Contrast given by $\delta C = C_2 - C_1$

Expand effective elastic tensor in a Taylor Series with respect to contrast

W.F. Brown (1955)

$$C^E = C_2 + \sum_{j=1}^{\infty} A_j (\delta C)^j$$

The geometry is encoded in the coefficients $A_j$, these are given in terms of N-point correlation functions.
One and two point correlation functions

One point correlation

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

Two point correlation

Probability that both ends of a segment lies in yellow phase when thrown into composite randomly
N-point correlation functions

N-point correlation function = probability that N points chosen at random lie inside yellow phase

An example of three point correlation.

Probability that all vertices of a triangle lies in yellow phase when thrown into composite randomly
One, two, and three-point correlation Functions

These statistical functions can be computed using techniques from image analysis. J. Berryman 1988.
Coefficients $A_j$ of contrast expansion

Set $\delta C(y) = C_1 - C_2$, for $y$ in material one

$\delta C(y) = 0$, for $y$ in material two

Set $e^0(y) = \bar{\varepsilon}$

And iterate according to

$$\text{div}(C_2 e^{j+1}(y)) = -\text{div}(\delta C(y) e^j(y)), j = 0, 1, 2, \ldots$$

And for $j = 1, 2, \ldots$ set

$$A_j \bar{\varepsilon} = \int_Q \delta C(y) e^j(y) \, dy$$

$A_j$ is given in terms of the $j$-point correlation function

W.F. Brown (1955), M. J. Beran (1965)
An Example: Bulk modulus for isotropic effective elastic tensor

\[ \delta \kappa = \kappa_2 - \kappa_1 \]
\[ \delta \mu = \mu_2 - \mu_1 \]

\[ \kappa^E = \kappa_2 + \delta \kappa A_1 + (\delta \kappa)^2 A_2 + (\delta \kappa)^3 A_3^1 + \delta \mu (\delta \kappa)^2 A_3^2 \]

\[ A_1 = \theta \]
\[ A_2 = -\frac{3\theta(1-\theta)}{\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)} \]
\[ A_3^1 = \frac{9\theta(1-\theta)(1-2\theta)}{[\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)]^2} \]
\[ A_3^2 = \frac{12\theta(1-\theta)(\zeta_1 - \theta)}{[\theta(3\kappa_1 + 4\mu_1) + (1-\theta)(3\kappa_2 + 4\mu_2)]^2} \]

Here \( \zeta_1 \) is a geometric parameter given in terms of the three point correlation function

\[ 0 \leq \zeta_1 \leq 1 \]
The parameter $\zeta_1$ is computed for cubic arrays of spheres in McPhedran and Milton (1981).

Extensive references to the literature and detailed analysis can be found in the recent books by G. Milton (2002) and S. Torquato (2002).
Bounds on effective properties: An example from heat conduction inside composite media

Consider the ensemble of composite samples made from two isotropic heat conductors with same volume fractions – having an isotropic effective conductivity \( \Sigma^E = \sigma^E I \).

Subject each sample to the same imposed temperature gradient.

Find lower and upper bounds on the effective thermal conductivity \( \sigma^E \).

Identify realizations that attain the bounds.
Setting

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

Conductivities: $\sigma_1 > \sigma_2$

Volume fractions: $\theta_1, \theta_2$

$\Delta T = 0$  \hspace{1cm} Inside each phase

$n \cdot \sigma_1 \nabla T = n \cdot \sigma_2 \nabla T$  \hspace{1cm} On interface

$\langle \nabla T \rangle = E$  \hspace{1cm} and  \hspace{1cm} $T - E \cdot x$  \hspace{1cm} is periodic on the cube
Effective Conductivity

\[ \sigma(y) \] is the local conductivity taking the value \( \sigma_1 \) inside material one and \( \sigma_2 \) inside material two.

The effective conductivity is given by

\[
\sum^e E = \int_Q \sigma(y) \nabla T(y) dy
\]
 Bounds of Hashin and Shtrikman for effective properties

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

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

\[ \sigma^e \leq \sigma_1 + \frac{3 \theta_2 \sigma_1 (\sigma_2 - \sigma_1)}{3 \sigma_1 + \theta_1 (\sigma_2 - \sigma_1)} \]
Coated sphere assemblage of Hashin and Shtrikman

Step I: Fill the RVE with a sphere packing with sphere sizes ranging to the infinitesimal.

Step II: Place a smaller concentric sphere inside each sphere such that the ratio of the radii of the outer and inner spheres is the same.
Optimal Microgeometries

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

The upper bound is attained by the Hashin Shtrikman coated sphere assemblage with core of material two and coating of material one.
Bounds for effective thermal conductivity with coupled mass and thermal transport on the two-phase interface

Green spheres represent pores
Matrix is ceramic

Physical Process:
A temperature gradient is placed across porous ceramic
Impurities diffuse through matrix and release heat when arrive on surface of pore.
When impurities the leave pore surface and reenter matrix they absorb heat; this effect can enhances or decrease the effective conductivity of the porous ceramic.
Steady state coupled heat and mass transport inside the RVE

Thermal conductivity of the matrix $\sigma_m$
Thermal conductivity of the pore $\sigma_p: \sigma_p < \sigma_m$
Temperature inside the composite $T = T(y)$
Impurity concentration inside the composite $C = C(y)$
Impurity concentration on the pore surface $C_s = C_{so} + \alpha_T (T - T_0) + \alpha_C (C - C_0)$
$C_{so}, T_0, C_0$ are the equilibrium values and $\alpha_T = \frac{\partial C_s}{\partial T}_{c_0, T_0}$, $\alpha_C = \frac{\partial C_s}{\partial C}_{c_0, T_0}$

The surface diffusivity $a_s$ has dimensions of length x diffusivity
The coefficient $a_T$ is negative since $C_s$ decreases with temperature

$\Delta T = 0$ $\Delta C = 0$ inside each phase

$n \cdot (\sigma_m \nabla T)_{\text{matrix}} - n \cdot (\sigma_p \nabla T)_{\text{pore}} = -q D n \cdot \nabla C$ $\nabla_S \cdot (a_s \nabla_S C_s) = -D n \cdot \nabla C$

$q$ is specific heat release
Prescribed average temperature gradient $\mathbf{E}$
Boundary conditions: $T - \mathbf{E} \cdot \mathbf{x}$ is $Q$ periodic, $C$ is $Q$ periodic.
Effective thermal conductivity

\[ E \]

Prescribed average temperature gradient across RVE

\[ j \]

Prescribed average heat flux across RVE

\[ j = \sum^E E \]
Microgeometry known only statistically

It is supposed that the microgeometry is such that the effective conductivity is an isotropic tensor $\Sigma^E = \sigma^E I$.

The microgeometry is composed of spherical pores of different radii. It is supposed that the volume fraction and size distribution of pore phase is known.

*Since the matrix is a better conductor than the pore we seek to determine conditions on the pore size distribution and material properties for which $\sigma^E > \sigma_m$ and $\sigma^E < \sigma_m$*

The effective conductivity with pore phase conductivity being perfect conductor is $\sigma^\infty$. The effective conductivity with pore phase insulator is and $\sigma^0$. 
Interplay between microgeometry and material properties

Average pore radii $\langle a \rangle$

Harmonic average of pore radii $\langle a^{-1} \rangle^{-1}$

If

$$\langle a^{-1} \rangle^{-1} \geq \frac{-2q a_s a_T}{\sigma_m - \sigma_p} - 2a_s \frac{a_c}{D} \left( \frac{\sigma^\infty - 1}{\theta_p} - 1 \right)^{-1}$$

Then

$$\sigma^E \leq \sigma_m$$

No enhanced conduction for sufficiently small surface to volume ratio

If

$$\langle a \rangle \leq \frac{-2q a_s a_T}{\sigma_m - \sigma_p} - 2a_s \frac{a_c}{D} \left( \frac{1 - \sigma^0}{\theta_p} - 1 \right)$$

Then

$$\sigma^E \geq \sigma_m$$

Enhanced conduction for surface to volume ratio sufficiently large

R. Lipton (1999)
JMPS (47)1699-1736
One has upper and lower bounds on $\sigma^\infty$ and $\sigma^0$ in terms of a lower bound on particle separation, Bruno (1991) P. Roy. Soc. Lond. (433) 355-381.

For monodisperse suspensions see Torquato and Rubinstein J. App. Phys. (69) 7118-712 for bounds on $\sigma^\infty$ and $\sigma^0$ in terms of nearest neighbor distribution function.