Influence of Pore Morphology on Mechanical Properties of Second Gradient Materials

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Homogenization translates behaviour of heterogeneous materials from the microscale level to the macroscale level. Most of the natural or man made materials are heterogeneous at some scale.
 Knowledge Gap

- Homogenization methods typically account for volume fractions and do not consider microscopic morphology and their impact on material behaviour.
- Effects of higher-order parameters are still under investigation and experimentally are challenging to measure.
- Microscopic impact is usually more challenging for multi-physics problems.

![Images of mesoporous colloidal SiO₂ samples](attachment:images.png)

Simulation method: Reactive molecular dynamics (RMD)
Simulation Tool: LAMMPS
\( q \) - SiO₂ (\( \rho = 2.2004 \text{ g/cm}^3 \))
\( T = 300 \text{ K}, P = 1 \text{ atm} \)
Strain rate = \( 5 \times 10^9 \text{ s}^{-1} \)
Boundary conditions: full periodic
Loading conditions: tension
Lx and Ly are varied
Vo and Newell 2020, Nanomaterials
Vo and Newell 2020, Computational Materials Science
Objectives

- Develop numerical framework capable of capturing higher-order homogenization parameters
- Investigate the role of pore/inclusion morphology (size, shape and distribution) on effective material properties
Methodology

Macroscale and microscale deformation energy of the RVE are equal:

\[
\int_{\Omega^p} \Phi^m dV = \int_{\Omega^p} \Phi^M dV
\]

Microscale
Macroscale

\(\Phi^m\) is expressed with first-order theory and \(\Phi^M\) with second-order theory:

First-order

\[
\int_{\Omega^p} \frac{1}{2} (C_{ijkl}^m u_{i,j}^m u_{j,i}^m) dV
\]

Second-order

\[
\int_{\Omega^p} \frac{1}{2} (C_{ijkl}^M u_{i,j}^M u_{j,i}^M + 2G_{ijklmn}^M u_{i,j}^M u_{k,l}^M + D_{ijklmn}^M u_{i,jk}^M u_{l,lm}^M) dV
\]
Methodology cont.

Macroscopic case is solved by evaluating deformation energy at the RVE’s geometric center as

\[ \dot{X} = \frac{1}{V} \int_{\Omega_p} XdV: \]

\[ \int_{\Omega_p} \Phi^M dV = \frac{V}{2} (C^{M}_{ijlm} \langle u^{M}_{i,j} \rangle \langle u^{M}_{i,m} \rangle + 2G^{M}_{ijklm} \langle u^{M}_{i,j} \rangle \langle u^{M}_{k,lm} \rangle) + (C^{M}_{ijlm} \bar{I}_{kn} + D^{M}_{ijklmn}) \langle u^{M}_{i,jk} \rangle \langle u^{M}_{l,mn} \rangle) \]

Microscopic case is solved through asymptotic homogenization method:

\[ u^m(X) = 0u(X, y) + \epsilon^1u(X, y) + \epsilon^2u(X, y) \]

\[ \epsilon = \frac{l}{L} = \frac{\text{microscale length}}{\text{macroscale length}} \]

Homothetic ratio

\[ y_j = \frac{1}{\epsilon} (X_j - \dot{X}_j) \]

Local coordinate

Expanded microscale displacement field
Equilibrium condition at microscale: \((C_{ijkl}^m u_{k,l}^m)_j + f_i = 0\) leads to:

\[
u_i^m(X, y) = u_i^M(X) + \epsilon \varphi_{abi} u_{a,b}^M(X) + \epsilon^2 \psi_{abci} u_{a,bc}^M(X)
\]

Recalculate microscopic deformation energy as follows:

\[
\frac{V}{2} \left( \bar{C}_{abcd} \langle u_{a,b}^M \rangle \langle u_{c,d}^M \rangle + 2 \bar{G}_{abcde} \langle u_{a,b}^M \rangle \langle u_{c,de}^M \rangle \right) + \bar{D}_{abcdef} \langle u_{a,bc}^M \rangle \langle u_{d,ef}^M \rangle
\]

Compare macroscale and microscale energies to extract \(C^M\), \(G^M\) and \(D^M\) leads to:

\[
C_{abcd}^M = \bar{C}_{abcd}
\]

\[
G_{abcde}^M = \frac{1}{2} \bar{G}_{abcde}
\]

\[
D_{abcdef}^M = \bar{D}_{abcdef} - \frac{\epsilon^2}{V} C_{abcd}^M \int_{\Omega} y_c y_j dV
\]
Numerical Implementation in FEniCS

START

CAD Model and Mesh
SALOME

Assign Material Parameters
Define boundary conditions

Set Solver Parameters

FEniCS Solver

Solve $\psi_{abci}$, compute $G^{M}_{abcde}$ $D^{M}_{abcdef}$

Solve $\varphi_{abi}$, compute $C^{M}_{abcd}$

FINISH

FEniCS Solver
Problem Definition

- **Material**: concrete with $E_{\text{concrete}} = 40 \, [GPa]$ and $\nu = 0.2$
- **Problem 1**: $E_{\text{inclusion}} = 0 \, [GPa]$ and Volume Fraction $= 0 \rightarrow 50$
- **Problem 2**: Volume Fraction $= 20\%$ and $E_{\text{inclusion}} = 0 \rightarrow 40 \, [GPa]$
- **RVE size**: square $a \times a$; $a = 1, 2, 3$

- Inclusion shape: circle, square, ellipse and triangle

- Inclusion distribution: single, uniform and random
Obtained $E_h$ is strongly influenced by the inclusion shape.
First-Order Parameters - Variation of $E_{\text{inclusion}}$

![Graph showing variation of $E_{\text{inclusion}}$ with shape influence.]

**Take away message**

Obtained $E_h$ is influenced by inclusion shape influence once $E_{\text{void}} < 0.5E_{\text{matrix}}$ and obtained stiffness matrix $C^M$ is cubic/orthotropic.
Higher-Order Parameters - Variation of $D_{111111}^M$

Take away message

Obtained $D_{111111}^M$ is influenced by pore shape and distribution.
Conclusions

1. First order parameter $C^M$ is strongly influenced by pore/inclusion shape and difference between properties of matrix and pore/inclusion.

2. Second order parameters $D^M$ and $G^M$ are influenced by size, shape and distribution of pores/inclusions.

3. Due to the sensibility of $C^M$ to the inclusion’s shape and property, tailored materials with specific microstructure can be designed for various engineering and scientific applications.
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