Double-Scale homogenization of a Rattan-Based Porous Ceramic for Bone Regeneration

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INTRODUCTION – Biomorphic Apatite: Why does it resemble Bone?

CORTICAL BONE STRUCTURE

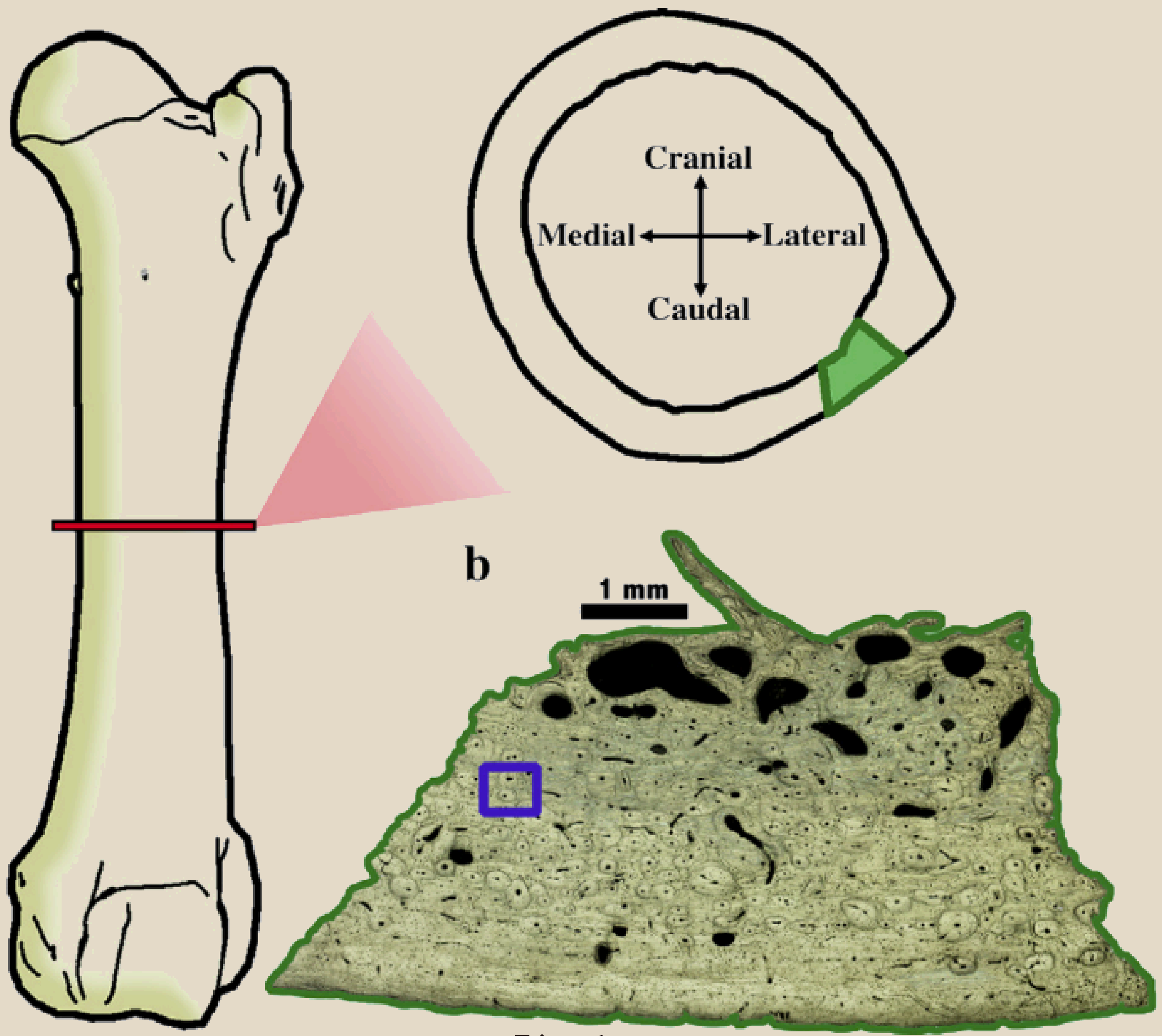


Fig.1

OSTEON

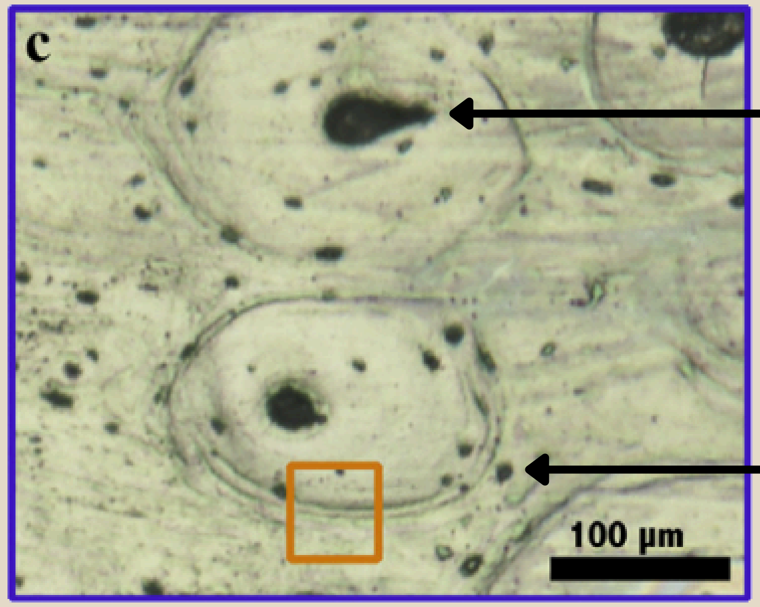


Fig.2

Haversian Canals:
Diameter ranges from **50–90** µm.

Osteocyte Lacunae:
Approximately **10-20** µm.

INTRODUCTION – Biomorphic Apatite: Why It Resembles Bone?

BIOMORPHIC APATITE (BA) STRUCTURE

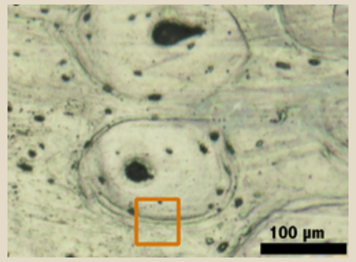


Fig.2

- **Haversian Canal: 50-90** µm.
- Osteocyte **lacunae: 10-20** µm.

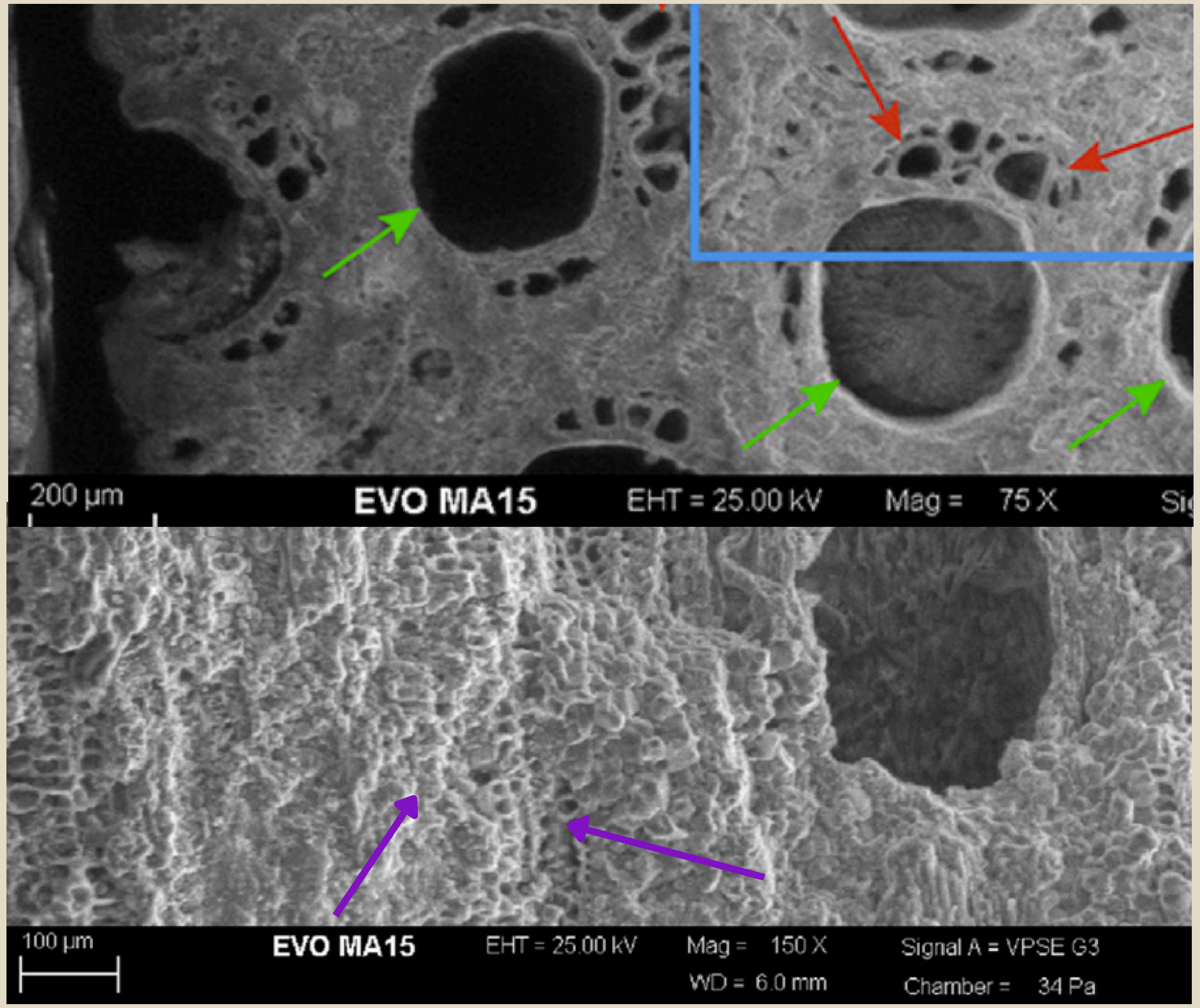


Fig.3- porosity at the 2 scales (SEM image) [3]

MESOSCALE

- Large **channel**: **200** µm. [1]
- Medium-sized **channels**: Up to **50** µm. [1]

MICROSCALE

- **Fine Porosity**: closed alveolar pores about **1** µm. [1]

INTRODUCTION - BA biomechanical properties

BA COMPOSITION

BA = Biomorphic Apatite =
= 95% hydroxyapatite(**HA**) + 5% **β-$Ca_3(PO_4)_2$** + other **bioactive** molecues

Property	HA	β-$Ca_3(PO_4)_2$	BA
Density	3.16 g/cm^3	3.07 g/cm^3	$0.95\times3.16 + 0.05\times 3.07 \approx$ **3.1555 g/cm^3**
Young Modulus	80-120 GPa	20-40 GPa	$0.95\times100 + 0.05\times30 \approx$ **96.5 GPa**

biocompatibility and osteoconductivity

damage tolerance

PROBLEM IDENTIFICATION - Literature data

POROSITY

ρ_sample = 1.47 g/cm^3 [1]

Φ_tot = ρ_sample / ρ_BA = 46.5%

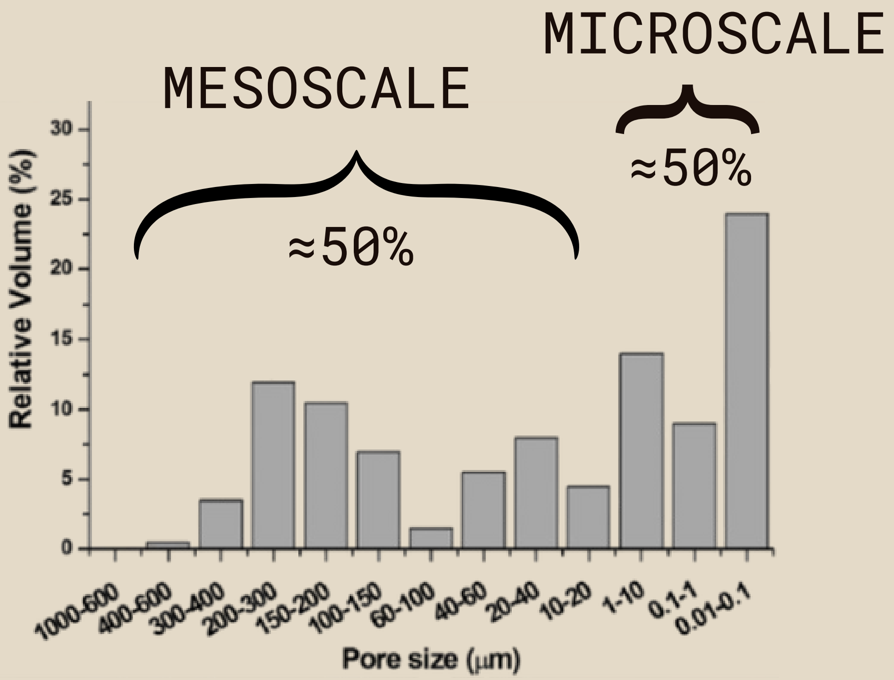
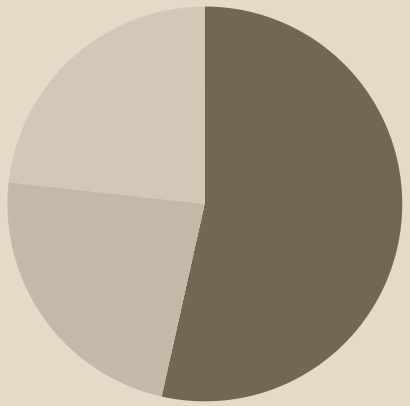


Fig.4 - Pore distribution [2]



Φ_meso = 23.25%/100% =

= **23.25%**

Φ_micro = 23.25%/(100-23.25)% =

= **30.5%** ⬆⬆⬆

PROBLEM IDENTIFICATION - Literature data

STIFFNESS

11 MPa (bending) < E_macro < 2800 MPa (ring compression)

Ultrasound testing $v_p = \sqrt{\frac{\lambda + 2\mu}{\rho}},$ $E = (\lambda + 2\mu) \cdot \frac{(1+\nu)(1-2\nu)}{(1-\nu)}$

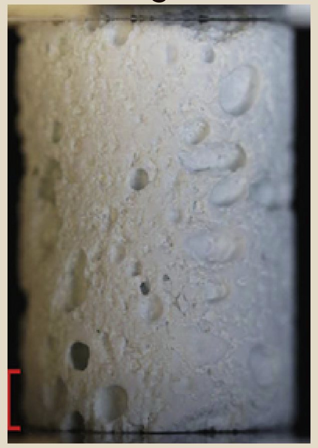
NON destructive

λ = 0.1–10 mm -> microscale pores **averaged out**

v_mesoscale = 0.25 -> **E_mesoscale = 8.665 Gpa**

PROBLEM IDENTIFICATION - Aim of the study

Fig.5



[1]

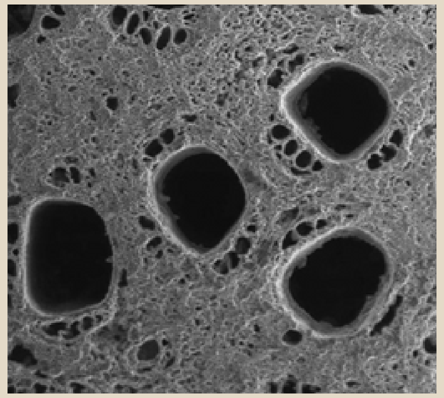
MACROSCALE

Young modulus

???

Mesoscale
homogenization

Fig.5



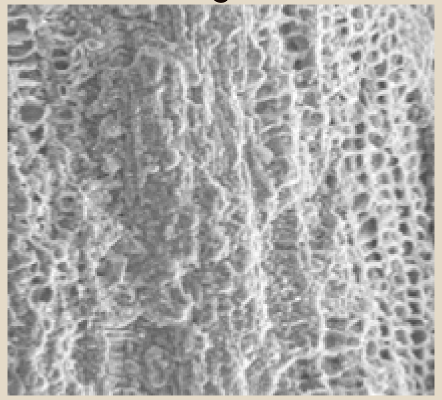
[1]

MESOSCALE

Young modulus
= 8.665 GPa

Microscale
homogenization

Fig.6



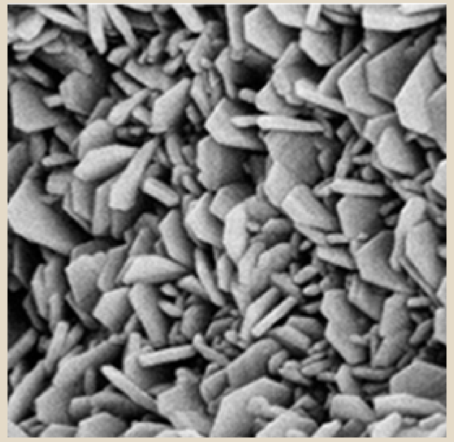
[1]

MICROSCALE

Young modulus

???

Fig.7



[2]

NANOSCALE

Young modulus
= 96.5 Gpa

MICROSCALE HOMOGENISATION - Mori-Tanaka method

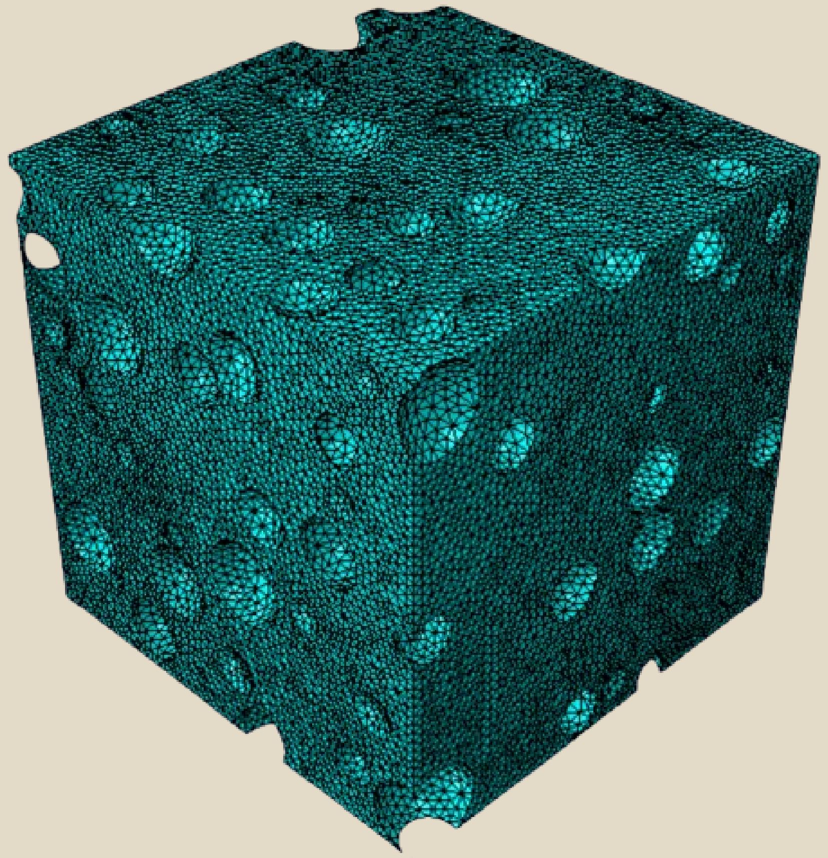


Fig.8

At the microscale, porosity main features are:

- **closed spheres** (do not touch each other)
- **random** spatial distribution
- spans from 0.01 to 10 μm
- **30.5%** of the total volume

Isotropic material assumption

MICROSCALE HOMOGENISATION - Mori-Tanaka method

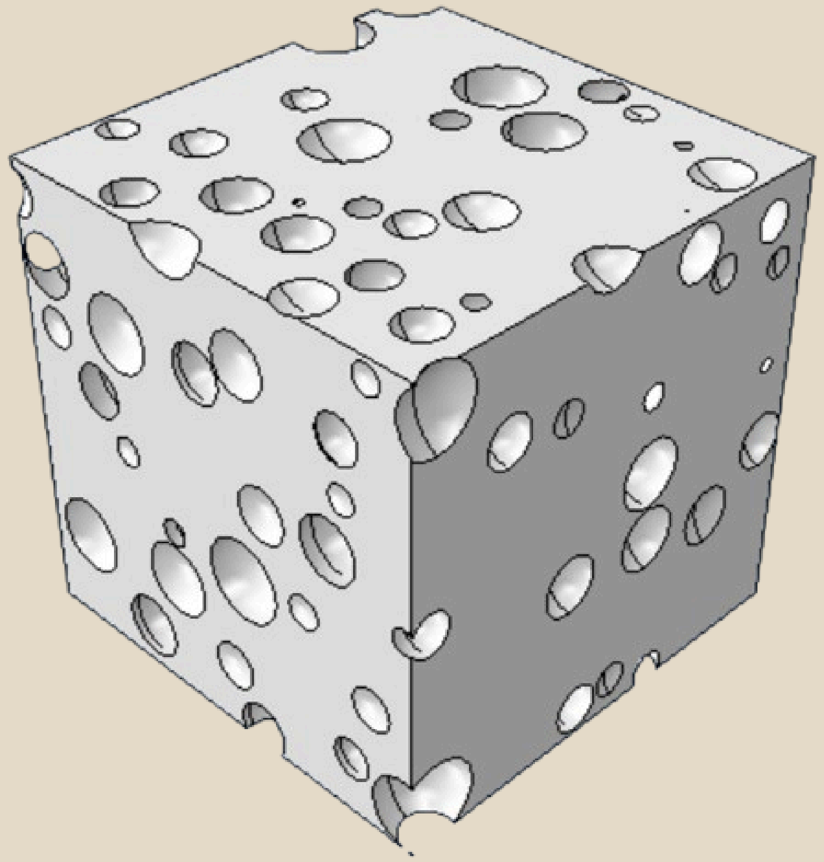


Fig.9

Matrix + **Soft inclusions**

E0 = few GPa ???
v0 = 0.3

K1 = 1e-6 Pa
G1 = 1e-6 Pa

Mesoscale
E = 8.665 GPa
v = 0.25

$$\bar{\mathbf{L}} = \mathbf{L}_0 + \underbrace{\sum_{r=1}^{N} c_r \left(\mathbf{L}_r - \mathbf{L}_0\right) \mathbf{T}_r \left[c_0 \mathbf{I} + \sum_{r=1}^{N} c_r \mathbf{T}_r\right]^{-1}}_{\text{inclusion-matrix interaction}}$$

»

$$\bar{K} = K_0 + \frac{c_1 K_0 \left(K_1 - K_0\right)}{K_0 + 3\gamma_0 \left(1 - c_1\right)\left(K_1 - K_0\right)}$$

$$\bar{\mu} = \mu_0 + \underbrace{\frac{c_1 \mu_0 \left(\mu_1 - \mu_0\right)}{\mu_0 + 2\delta_0 \left(1 - c_1\right)\left(\mu_1 - mu_0\right)}}_{\text{inclusion-matrix interaction}}$$

MICROSCALE HOMOGENISATION - Self Consistent method

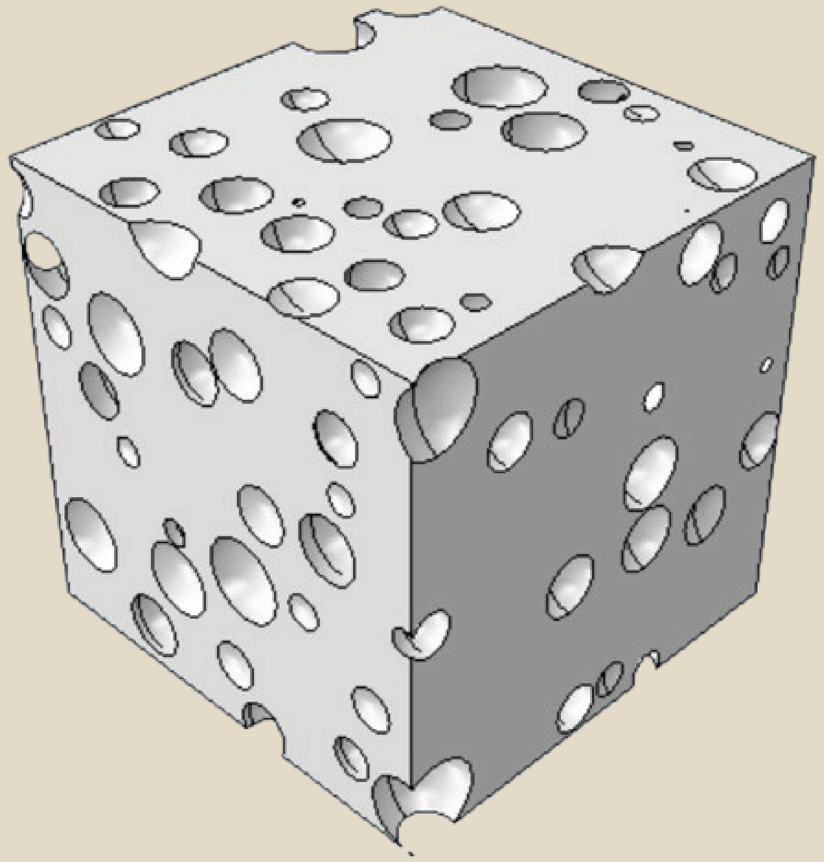
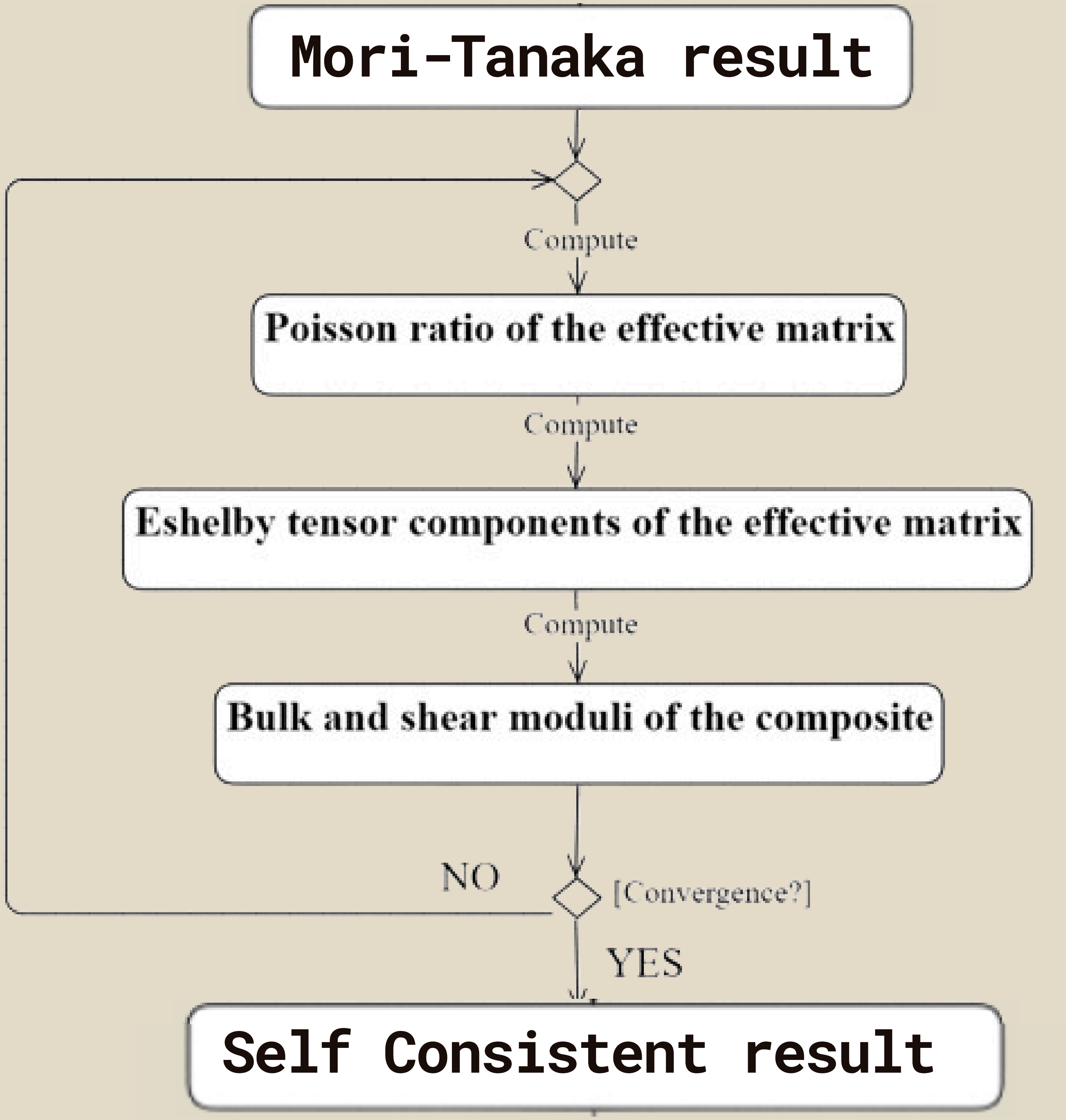


Fig.9

$$\bar{K} = K_0 + \frac{c_1 \bar{K}\left(K_1 - K_0\right)}{\bar{K} + 3\bar{\gamma}\left(K_1 - \bar{K}\right)};$$

$$\bar{\mu} = \mu_0 + \frac{c_1 \bar{\mu}\left(\mu_1 - \mu_0\right)}{\bar{\mu} + 2\bar{\delta}\left(\mu_1 - \bar{\mu}\right)}$$

inclusion-effective medium interaction



MICROSCALE HOMOGENISATION - Hashin-Shtrikman boundaries

Theoretical boundaries from a rivisited [3] Hashin-Shtrikman theory:

$$\underbrace{\left(\frac{\phi_1/2}{\frac{\delta-1}{\delta}\min[G_1,G_2]+K_1}+\frac{\phi_2/2}{\frac{\delta-1}{\delta}\min[G_1,G_2]+K_2}\right)^{-1}-2\frac{\delta-1}{\delta}\min[G_1,G_2]}_{\text{k\_min}} \leq K \leq \underbrace{\left(\frac{\phi_1/2}{\frac{\delta-1}{\delta}\max[G_1,G_2]+K_1}+\frac{\phi_2/2}{\frac{\delta-1}{\delta}\max[G_1,G_2]+K_2}\right)^{-1}-2\frac{\delta-1}{\delta}\max[G_1,G_2]}_{\text{k\_max}} \quad [3]$$

$$\underbrace{\left(\frac{\phi_1}{H_{\min}+G_1}+\frac{\phi_2}{H_{\min}+G_2}\right)^{-1}-H_{\min}}_{\text{G\_min}} \leq G < \underbrace{\left(\frac{\phi_1}{H_{\max}+G_1}+\frac{\phi_2}{H_{\max}+G_2}\right)^{-1}-H_{\max}}_{\text{G\_max}}$$

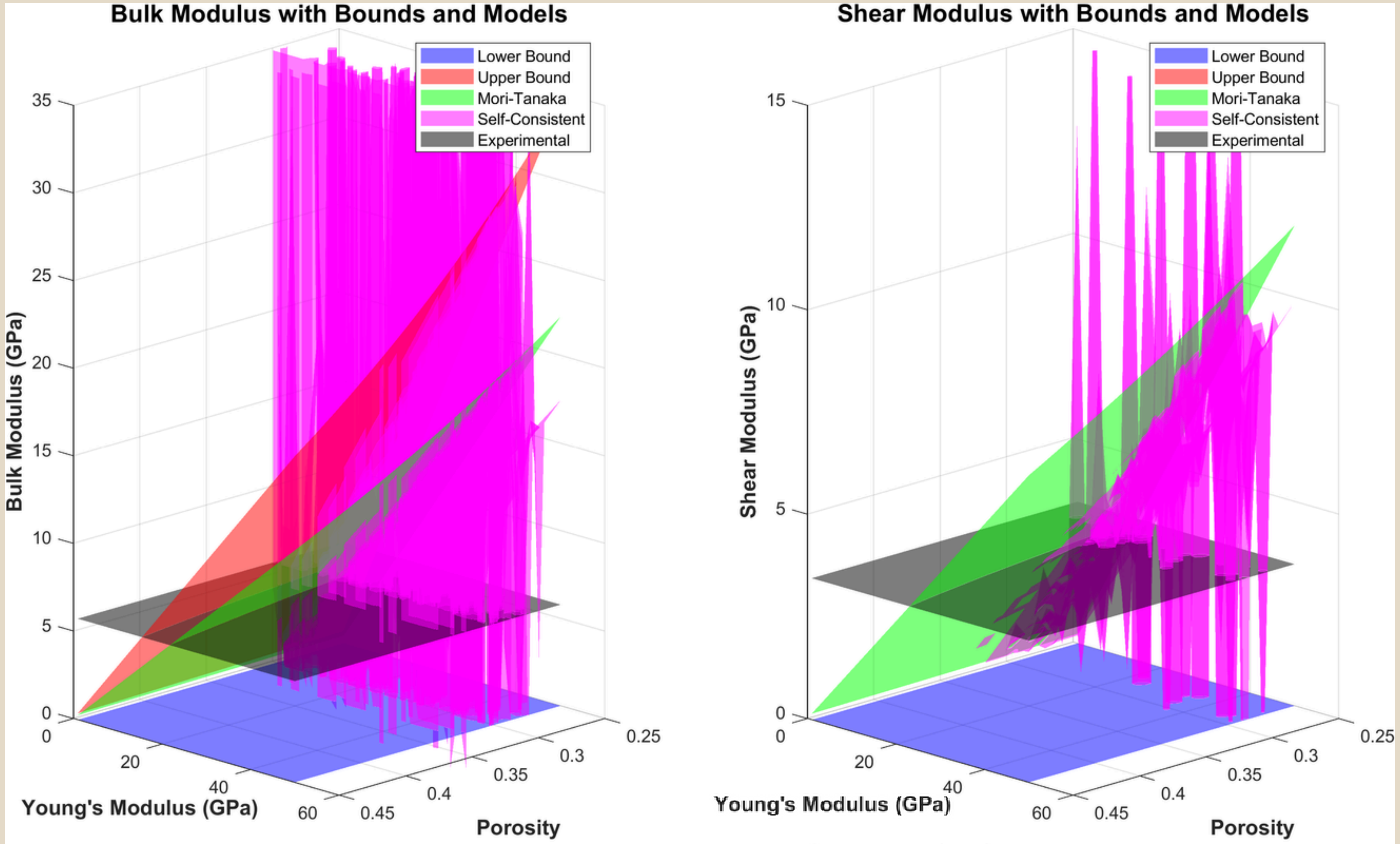
, where

$$H_{\min} = \begin{cases} G_2\dfrac{\delta K_2/2+(\delta+1)(\delta-2)G_2/\delta}{K_2+2G_2} & \text{if } G_1 \geq G_2 \\ G_1\dfrac{\delta K_1/2+(\delta+1)(\delta-2)G_1/\delta}{K_1+2G_1} & \text{if } G_1 < G_2 \end{cases}$$

$$H_{\max} = \begin{cases} G_2\dfrac{\delta K_2/2+(\delta+1)(\delta-2)G_2/\delta}{K_2+2G_2} & \text{if } G_2 \geq G_1 \\ G_1\dfrac{\delta K_1/2+(\delta+1)(\delta-2)G_1/\delta}{K_1+2G_1} & \text{if } G_2 < G_1 \end{cases} \quad [3]$$

MICROSCALE HOMOGENISATION - Results

Fig.10



Divergence

Infinite iterations

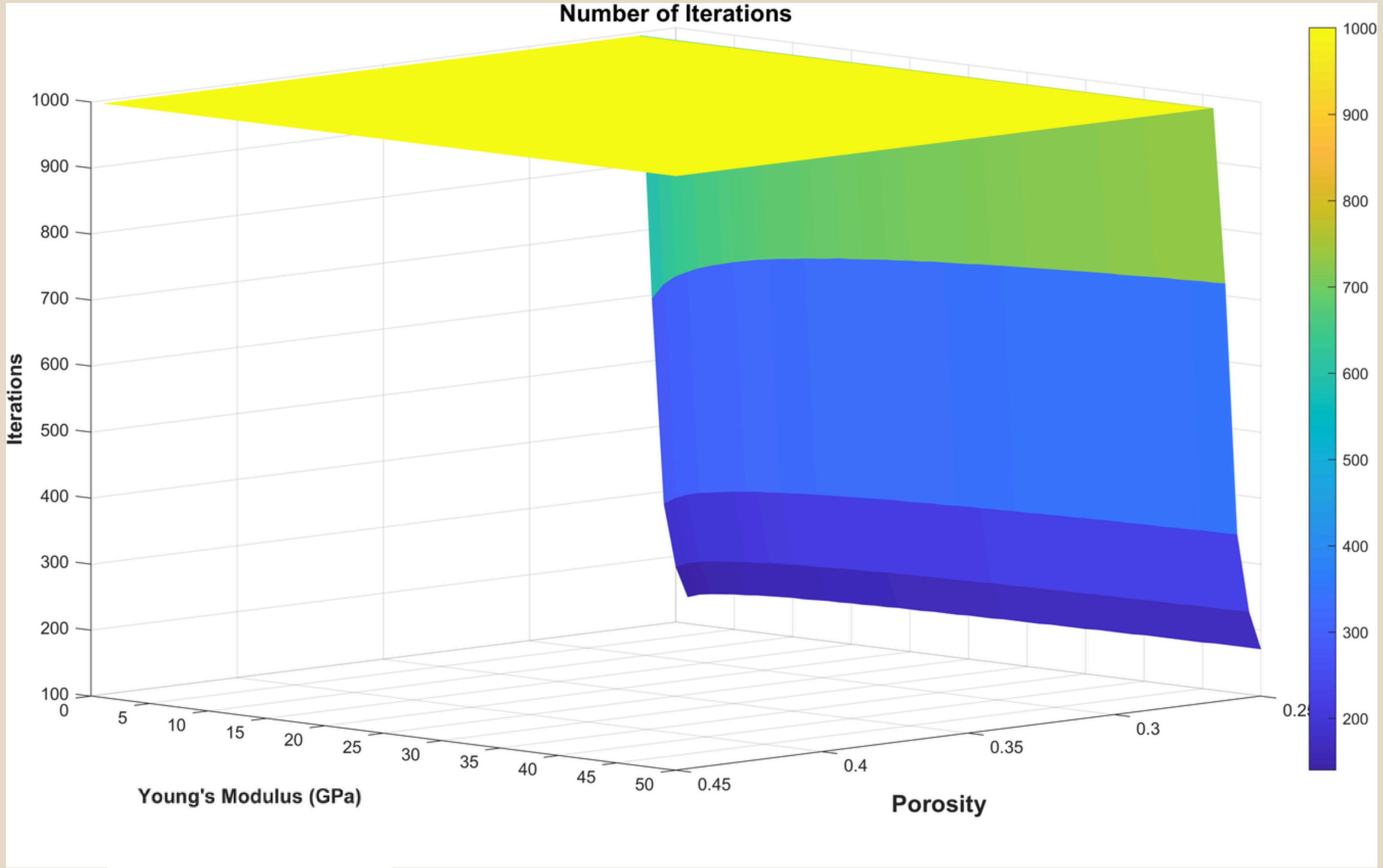


Fig.11

MICROSCALE HOMOGENISATION - Results analysis

```
% Update values for next iteration
K_SC = (1 - relax_factor) * K_SC + relax_factor * K_new;
G_SC = (1 - relax_factor) * G_SC + relax_factor * G_new;
```

Fig.13

Iteration count depends on:

- Stiffness mismatch
- Relaxation factor

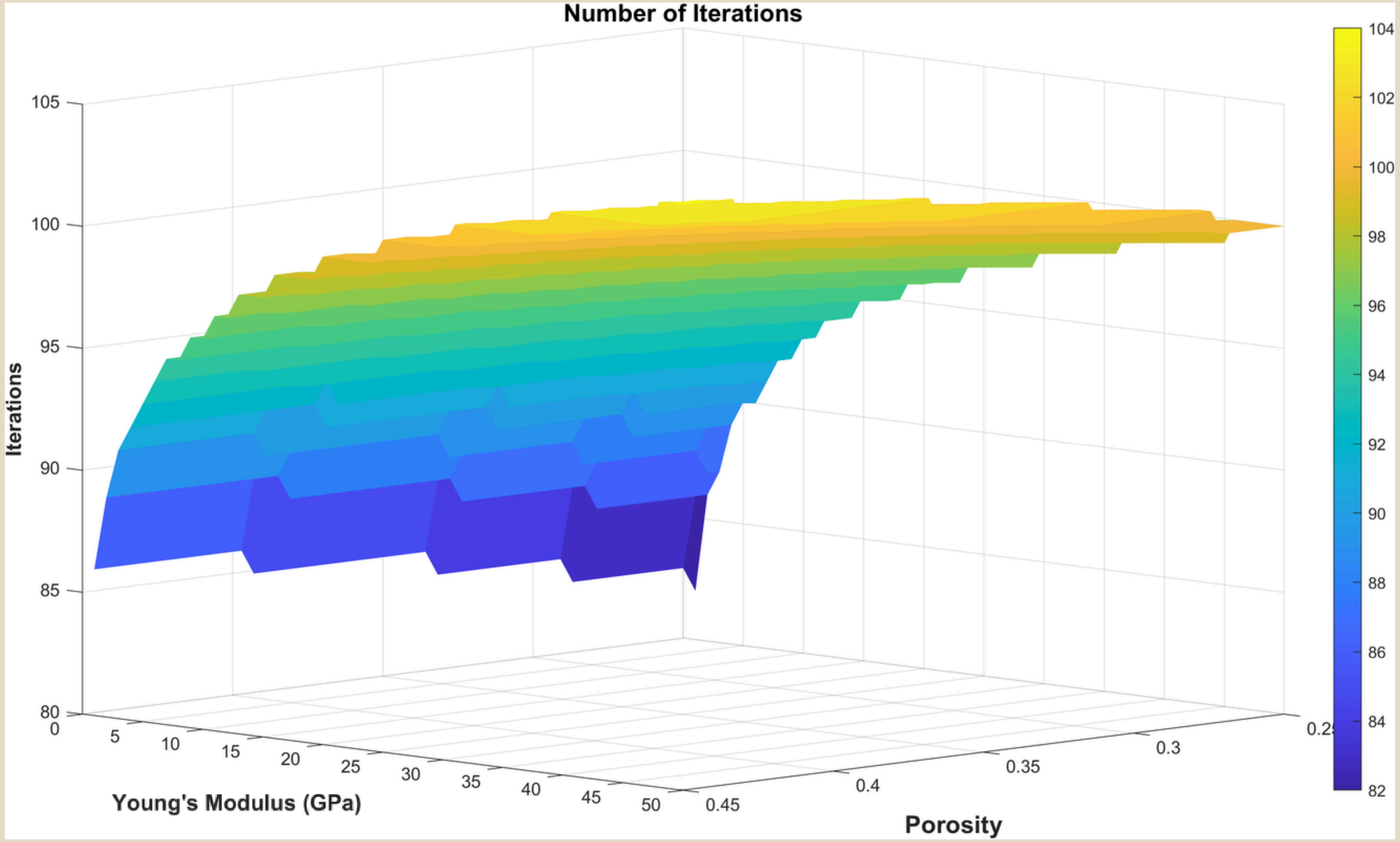


Fig.14

MICROSCALE HOMOGENISATION - Results analysis

```
% Update values for next iteration
K_SC = (1 - relax_factor) * K_SC + relax_factor * K_new;
G_SC = (1 - relax_factor) * G_SC + relax_factor * G_new;
```

Fig.13

MT overestimates the effective moduli

E_matrix is the intersection with experimental data

```
% Find the E_matrix that minimizes
% the total error between K_SC and G_SC
error_vals = abs(K_SC_vals - K_exp) +
             abs(G_SC_vals - G_exp);

[~, idx_best] = min(error_vals);

E_matrix = moduli(idx_best);
```

Fig.15

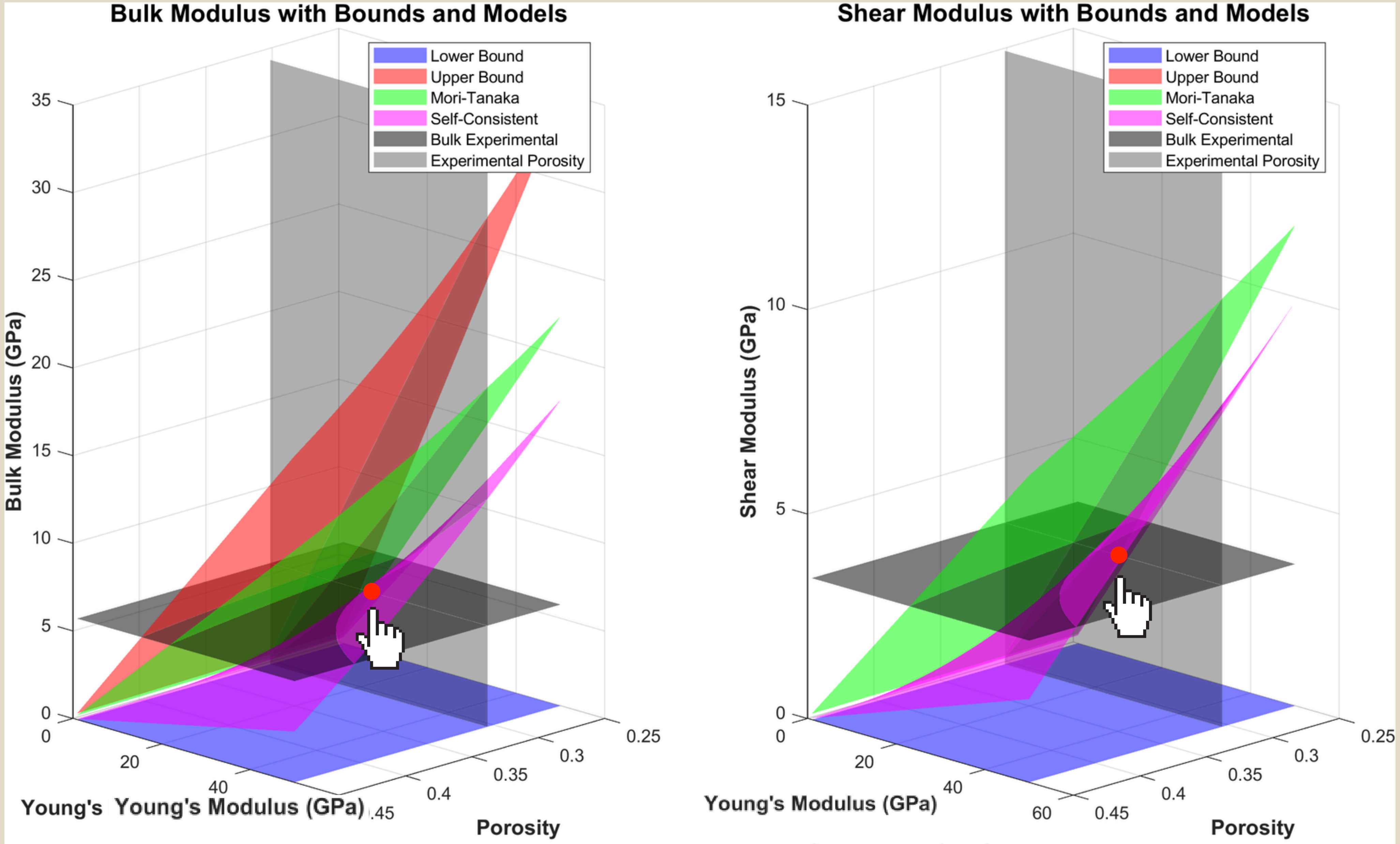
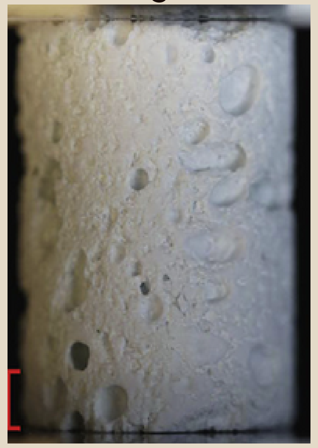


Fig.16

MICROSCALE HOMOGENISATION - Results analysis

Fig.5



[1]

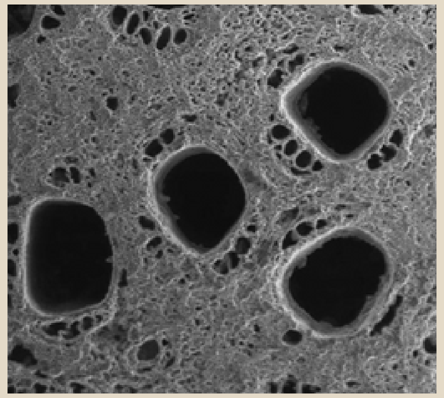
MACROSCALE

Young modulus

???

Mesoscale homogenization

Fig.5



[1]

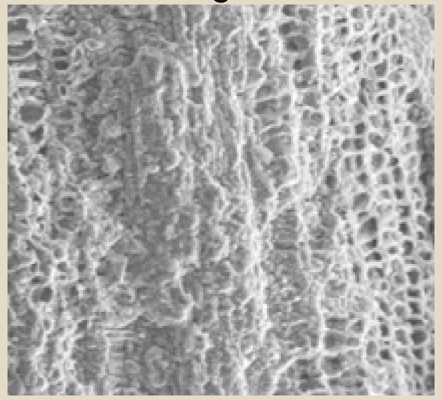
MESOSCALE

Young modulus

= 8.665 GPa

Mori-Tanaka

Fig.6



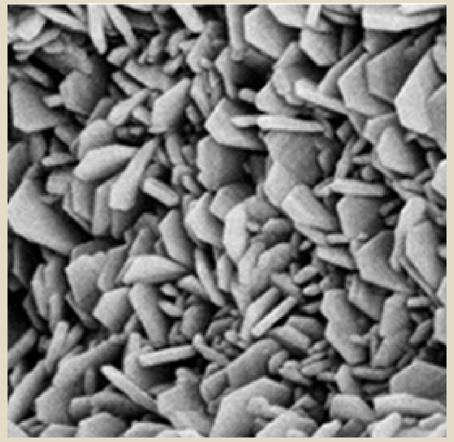
[1]

MICROSCALE

Young modulus

= 22.24 Gpa

Fig.7



[2]

NANOSCALE

Young modulus

= 96.5 Gpa

MESOSCALE HOMOGENISATION - RVE creation

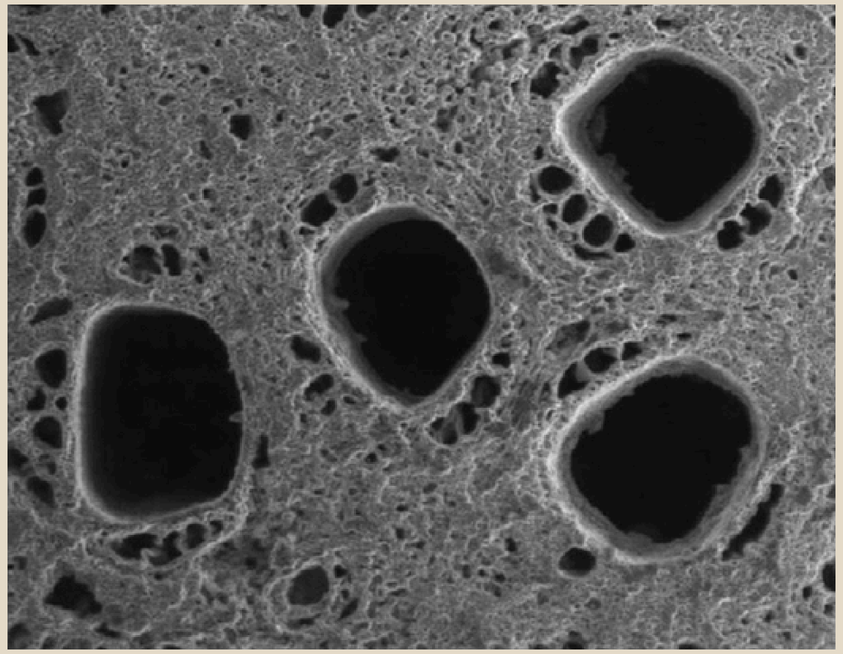


Fig.17 - x38 SEM image[1]

At the mesoscale, porosity main features are:

- **Irregular parallel cilindrical** shape
- **Random clustered** spatial distribution
- Spans from 10 to 300 μm
- **23.25%** of the total volume

Transverse isotropy assumption:

$$E = \begin{bmatrix} E_{xy} & 0 & 0 \\ 0 & E_{xy} & 0 \\ 0 & 0 & E_z \end{bmatrix}$$

MESOSCALE HOMOGENISATION - RVE creation

Transverse isotropy assumption: $$E = \begin{bmatrix} E_{xy} & 0 & 0 \\ 0 & E_{xy} & 0 \\ 0 & 0 & E_z \end{bmatrix}$$

Voigt to compute Ez: $$E_z = V_m E_m + V_p E_p \approx V_m E_m \quad \text{per} \quad E_p \to 0$$

$$E_z \approx (1 - 0.2325) \times 8.665 \text{ GPa} = 6.654 \text{ GPa}$$

2D finite element simulation using Periodic Boundary Conditions (**PBC**) to compute Exy: $$E_{xy} = \frac{E_x}{2} + \frac{E_y}{2}$$

MESOSCALE HOMOGENISATION - RVE creation

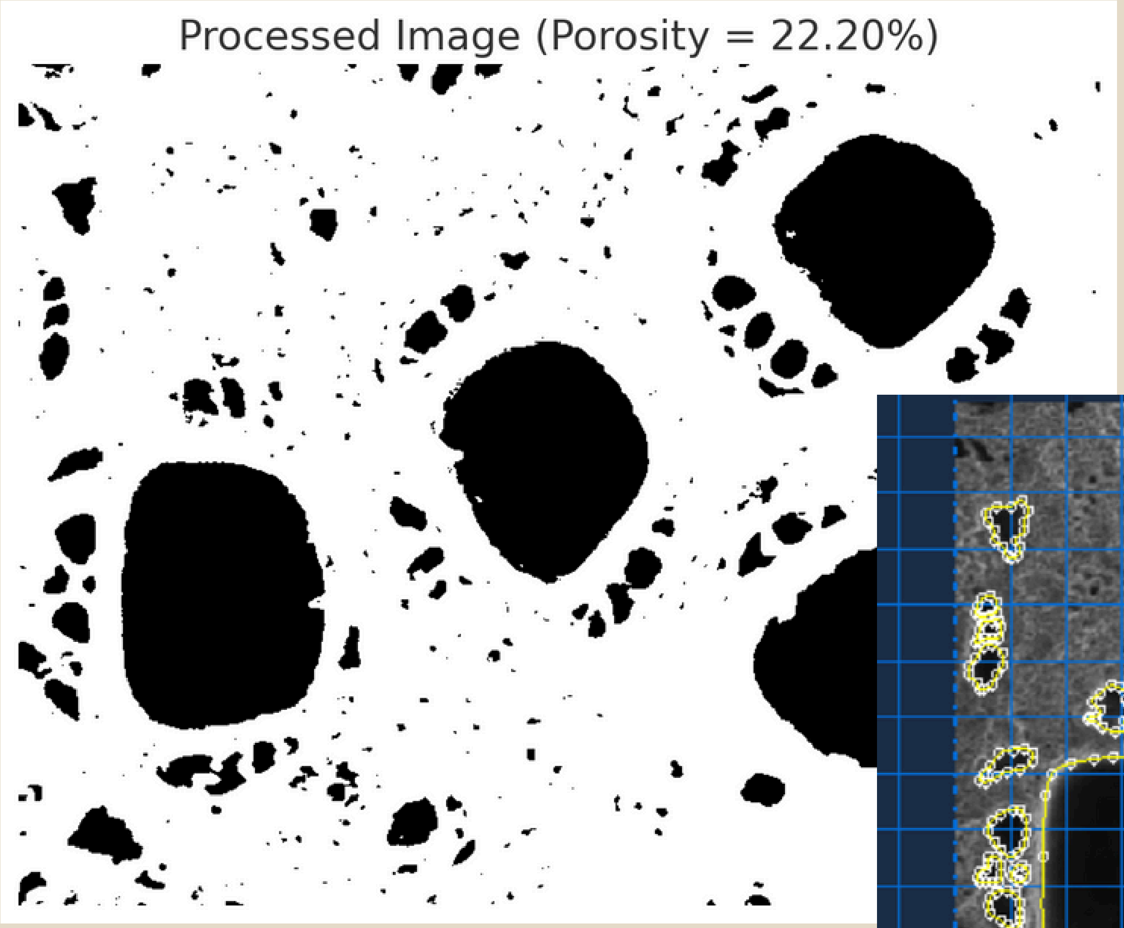


Fig.18

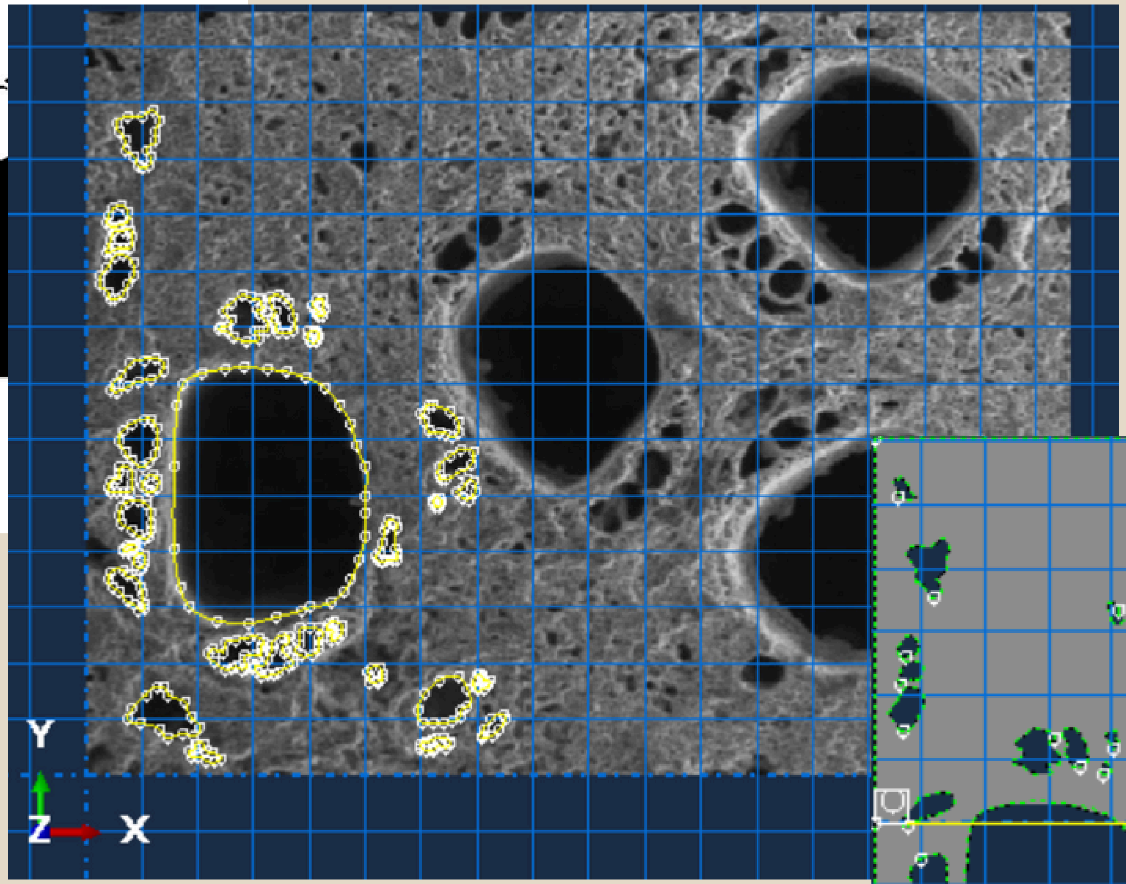


Fig.19

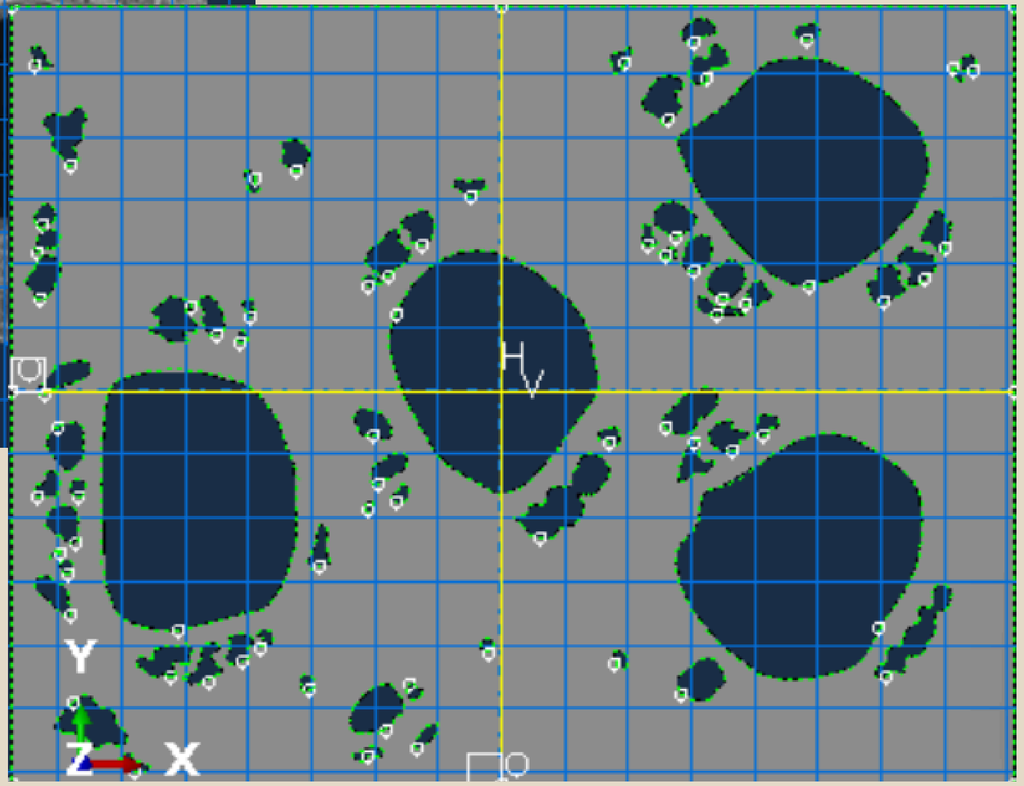


Fig.20

Porosity check

Sketch

Part

Partition

MESOSCALE HOMOGENISATION - RVE creation

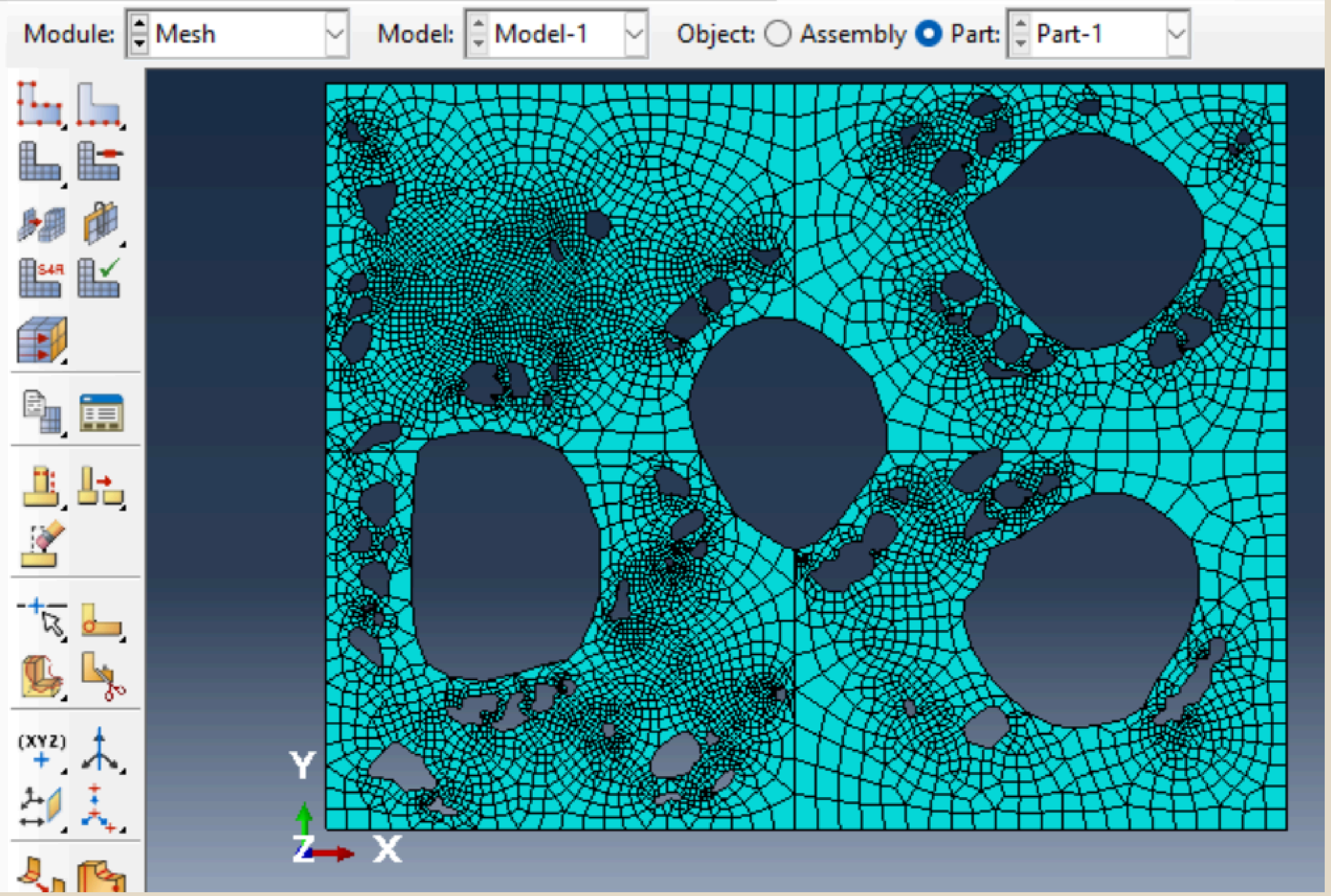


Fig.21

Meshing

Ensure node **Matching**

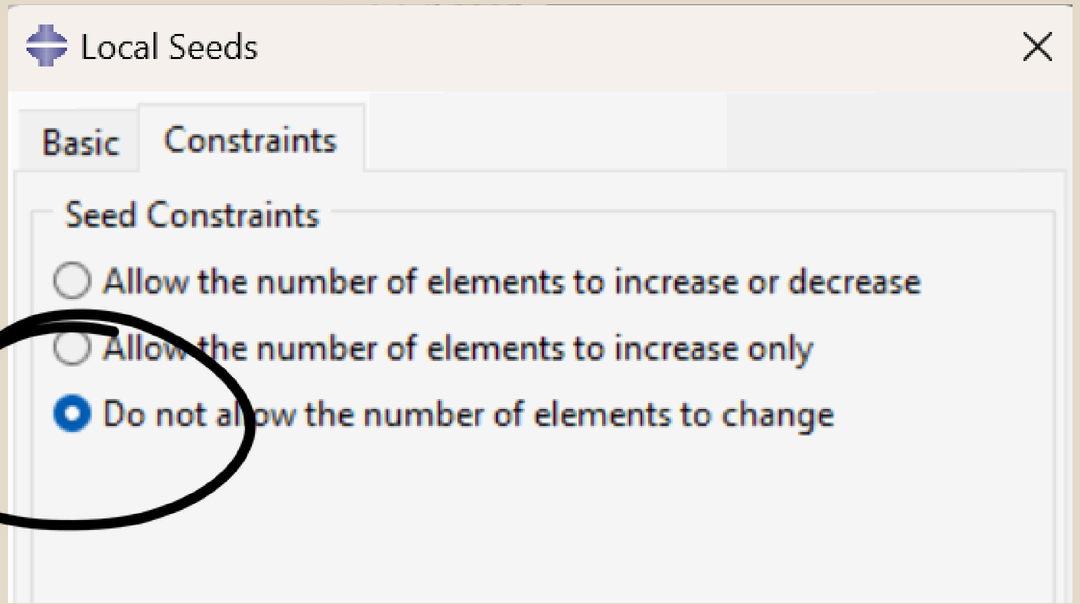


Fig.22

MESOSCALE HOMOGENISATION - Periodic Boundary Conditions(PBC)

Purely defined by **kynematic relations** (no load applied):

Equation $\mathbf{U}^{N_B}_{(x,y)} - \mathbf{U}^{N_A}_{(x,y)} = \mathbf{U}^{N_2}_{(x,y)} - \mathbf{U}^{N_1}_{(x,y)}$

Kynematic Constraints

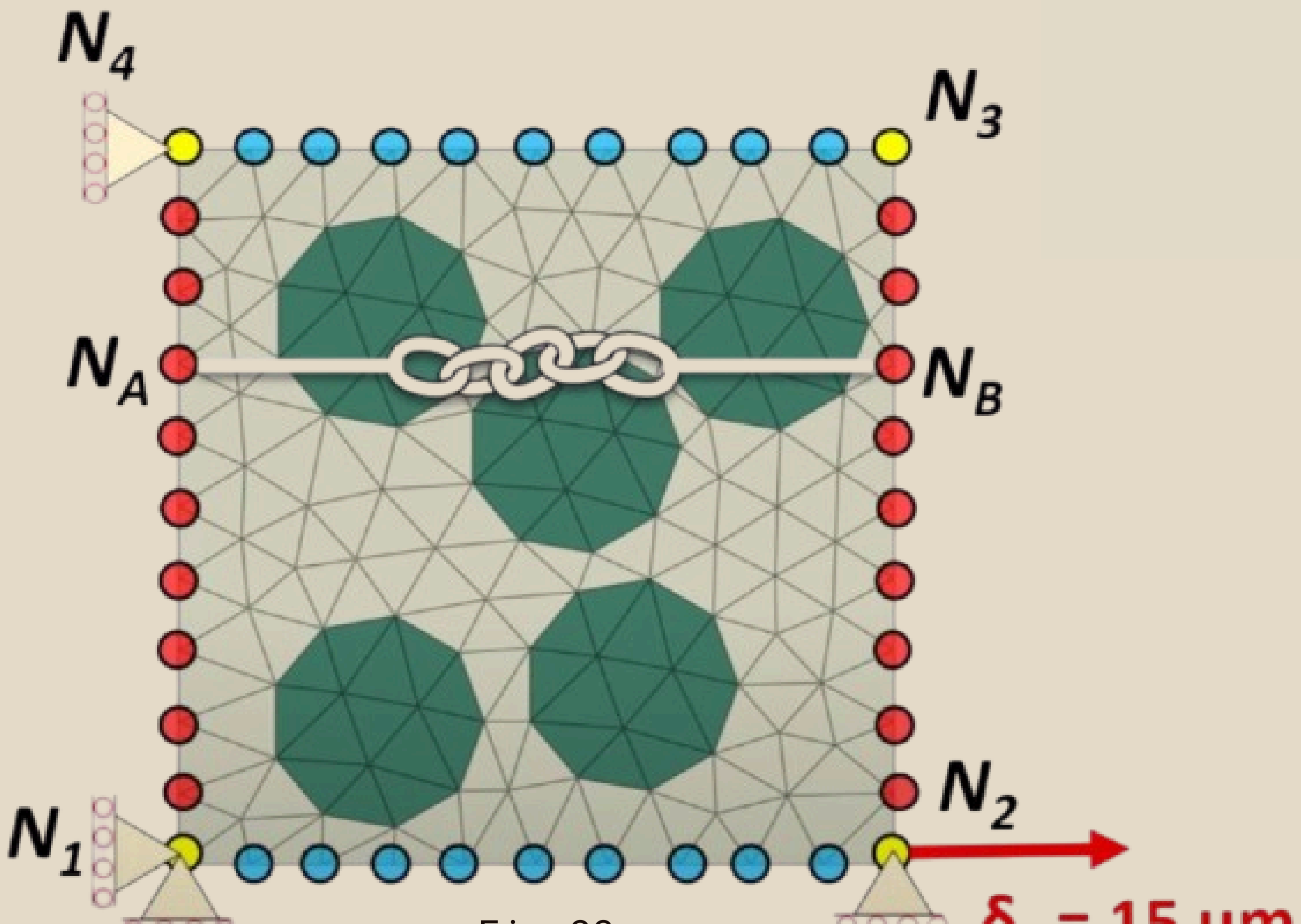


Fig.23

Displacement

MESOSCALE HOMOGENISATION - PBC

Average values $\boldsymbol{\sigma}_{\text{macro}} = \frac{1}{V}\int_V \boldsymbol{\sigma}(\mathbf{x})dV$ $\varepsilon_{\text{macro}} = \frac{1}{V}\int_V \varepsilon(\mathbf{x})dV$

Young Modulus $E = \frac{\sigma_{\text{macro}}}{\varepsilon_{\text{macro}}}$

Due to **PBC** $\varepsilon_{\text{macro}} = \frac{u_{\text{right}} - u_{\text{left}}}{L_0} = \frac{\Delta L}{L_0}$

MESOSCALE HOMOGENISATION - PBC

Cauchy stess theorem $\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}$

Gauss divergence theorem $\boldsymbol{\sigma}_{\text{macro}} = \frac{1}{V} \int_{\partial V} \mathbf{x} \otimes \mathbf{t} \, dA$

NO distributed Loading $\boldsymbol{\sigma}_{\text{macro}} \approx \frac{1}{V} \sum_i \mathbf{x}_i \otimes \mathbf{F}_i$ [4]

MESOSCALE HOMOGENISATION - PBC

```
*Equation
4
N303, 2, 1.
N312, 2, -1.
N290, 2, -1.
N291, 2, 1.
** -----------
```

Fig.23

Writing **equations** in the **input file**

Constraints (22)
- Eqn-1
- Eqn-2
- Eqn-3
- Eqn-4
- Eqn-5
- Eqn-6
- Eqn-7

Fig.24

Displacement and constraints

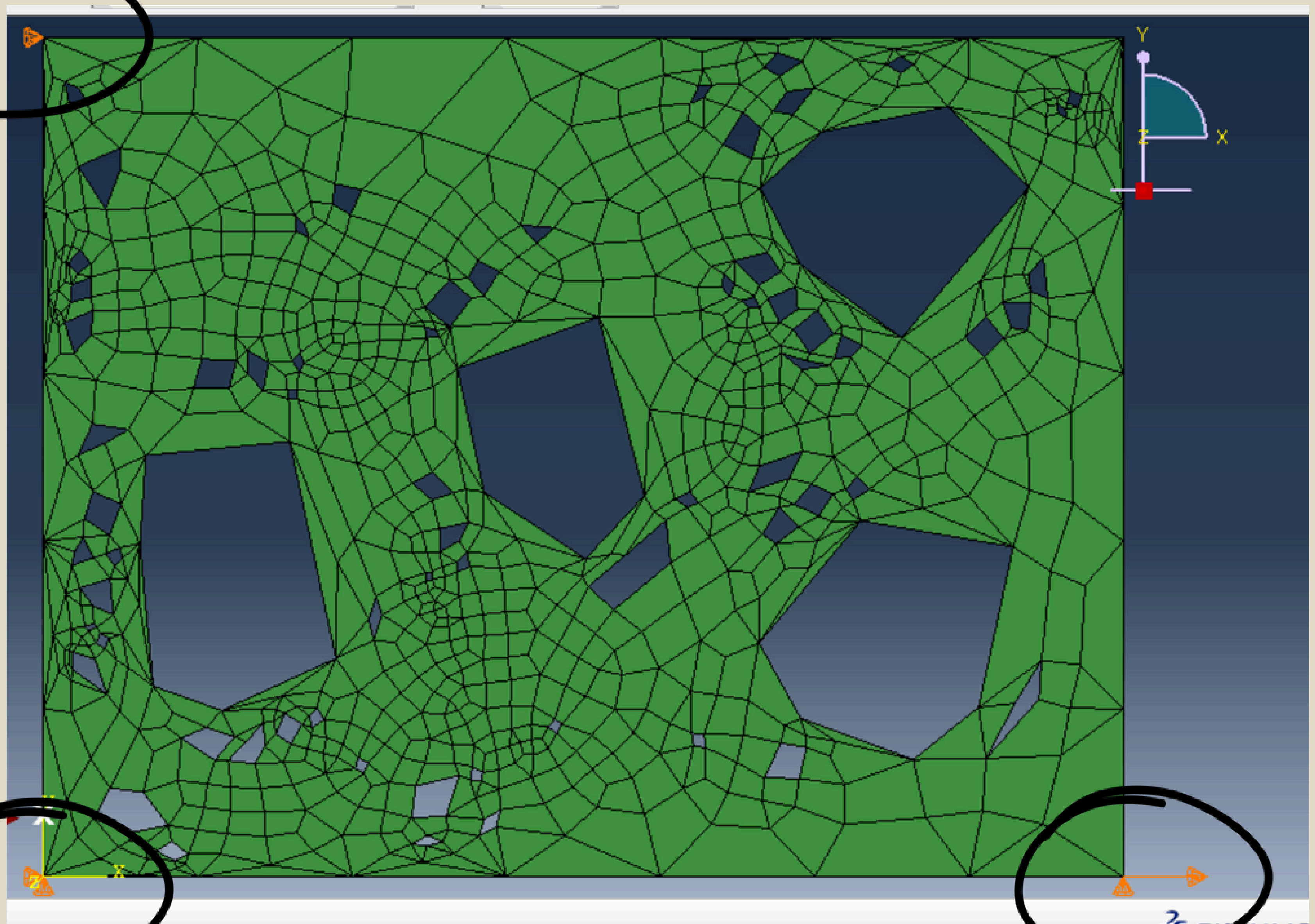


Fig.25

MESOSCALE HOMOGENISATION - PBC

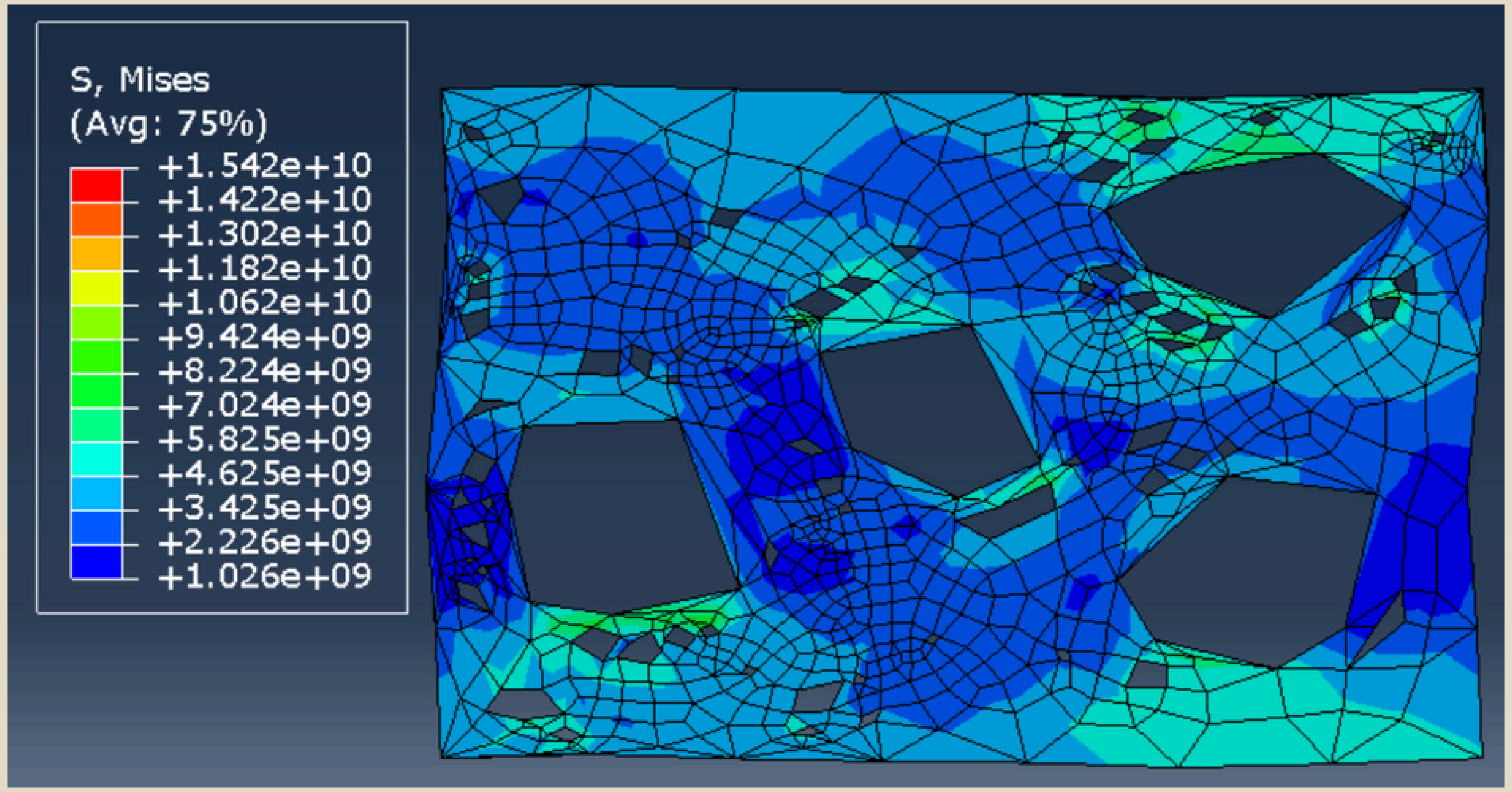


Fig.26

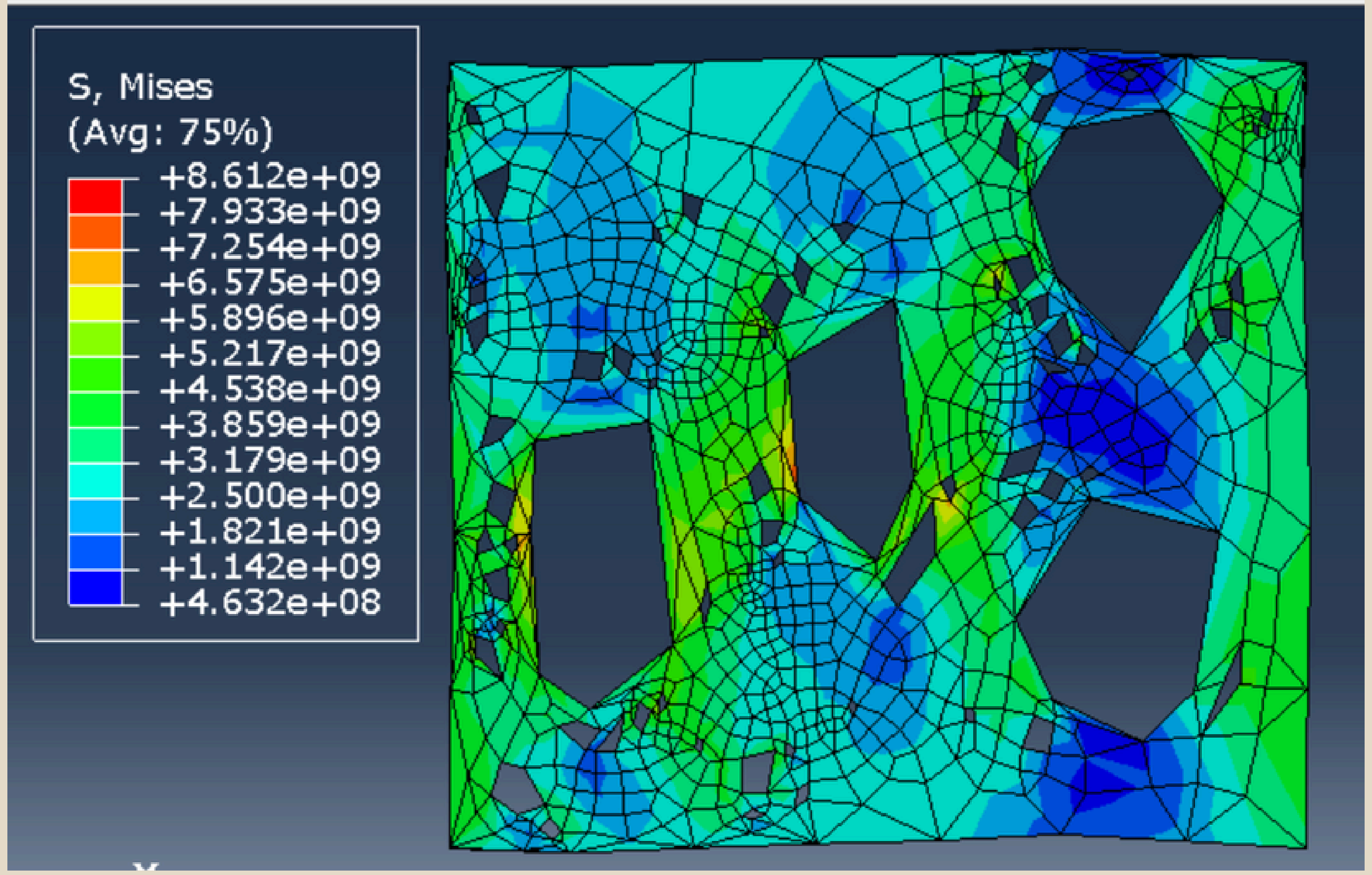


Fig.27

MESOSCALE HOMOGENISATION - RESULTS ANALYSIS

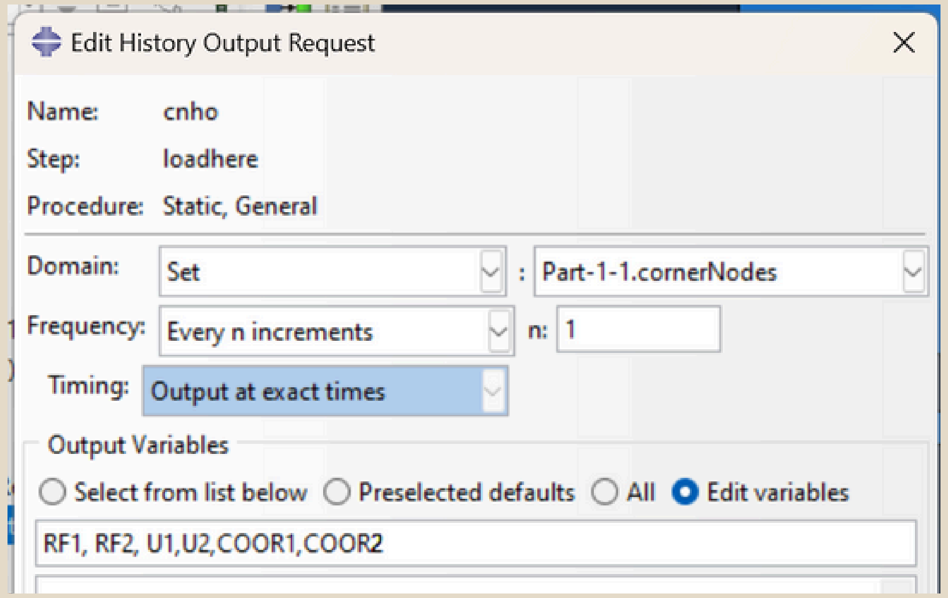


Fig.28

History **output**

Plotting

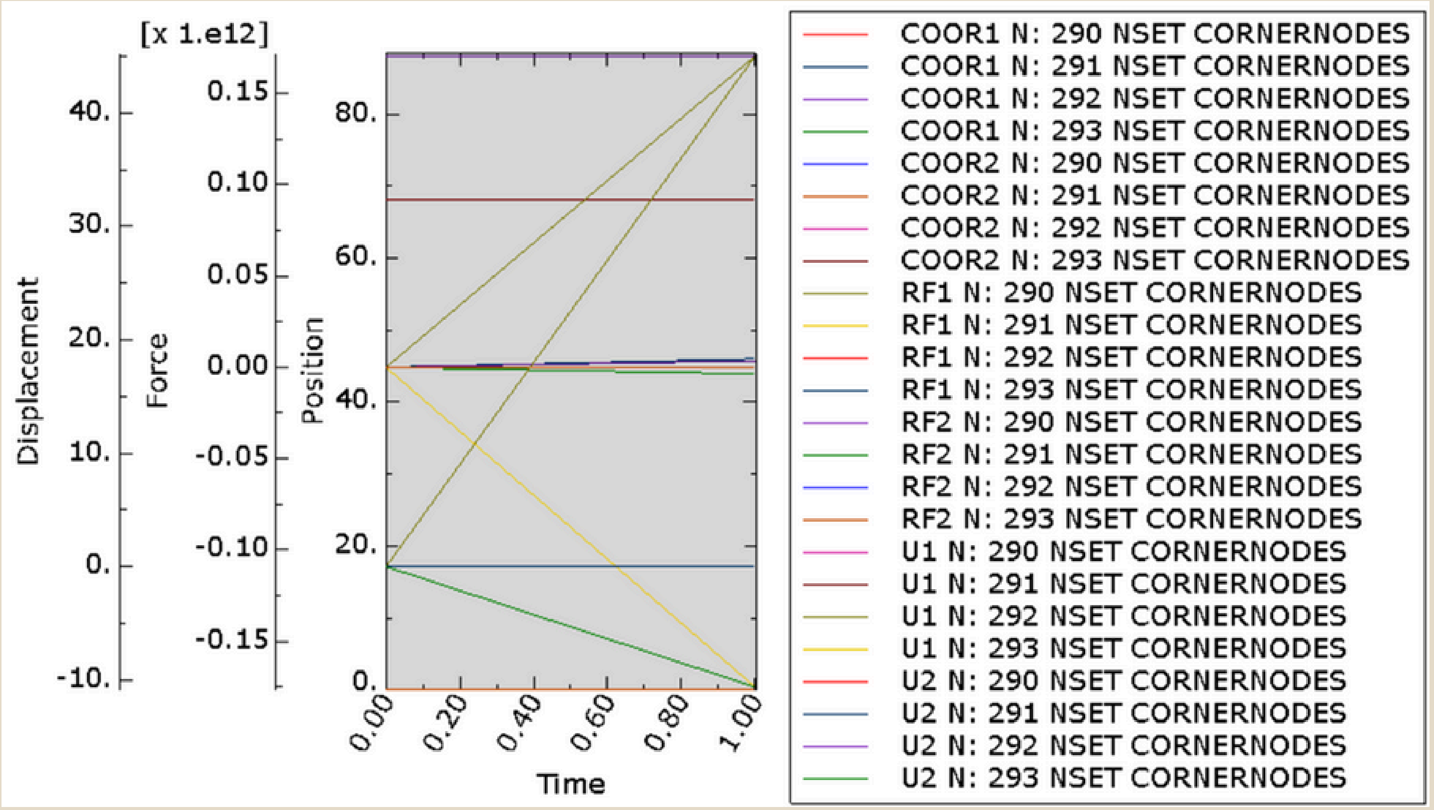


Fig.29

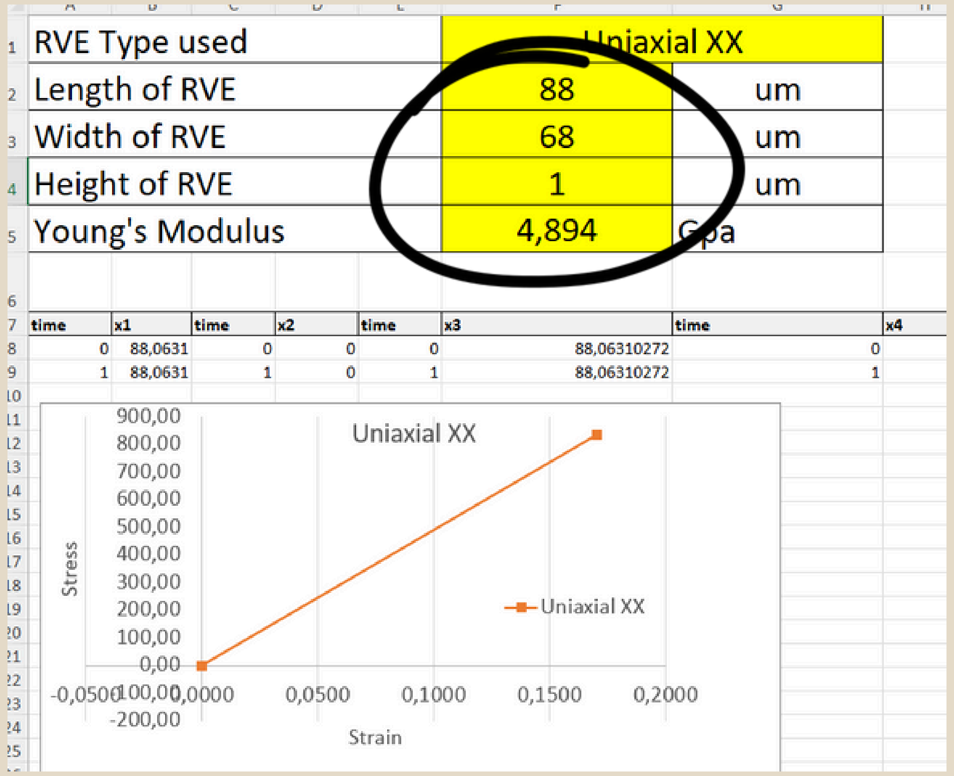
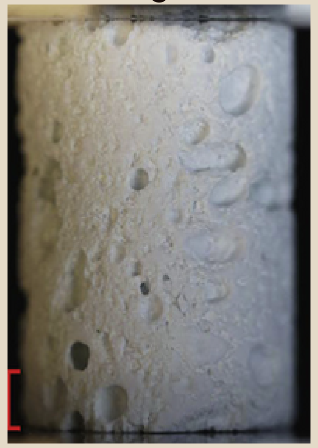


Fig.30

Post-processing on **EXCEL** to obtain **Ex = 4.8 GPa** and **Ey = 3.78 Gpa**

MESOSCALE HOMOGENISATION - RESULTS ANALYSIS

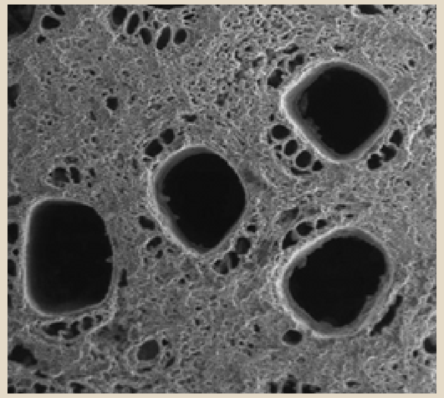
Fig.5



[1]

MACROSCALE

Fig.5



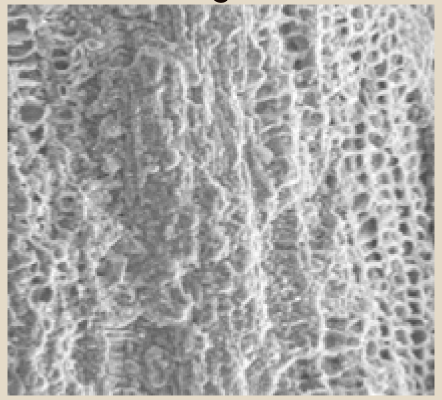
[1]

FEM simulation

MESOSCALE

Mori-Tanaka

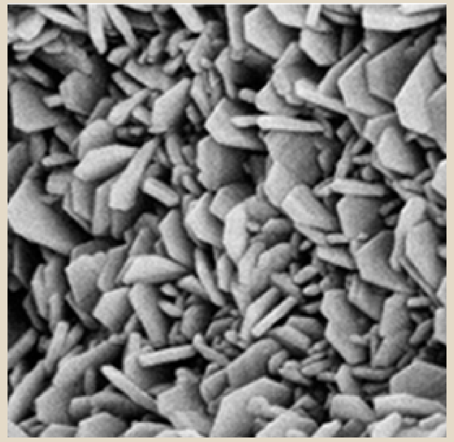
Fig.6



[1]

MICROSCALE

Fig.7



[2]

NANOSCALE

✓ **Young modulus**

$$\begin{bmatrix} 4.338 & 0 & 0 \\ 0 & 4.338 & 0 \\ 0 & 0 & 6.654 \end{bmatrix} \text{GPa}$$

✓ Young modulus = 8.665 GPa

✓ **Young modulus = 22.24 Gpa**

✓ Young modulus = 96.5 Gpa

MESOSCALE HOMOGENISATION - RESULTS ANALYSIS

- Ceramics with the signature of wood [1]
- Heterogeneous chemistry in the 3-D state: an original approach to generate bioactive, mechanically-competent bone scaffolds [2]
- Voigt-Reuss and Hashin-Shtrikman bounds revisited [3]
- Macroscopic stress, couple stress and flux tensors derived through energetic equivalence from microscopic continuous and discrete heterogeneous finite representative volumes [4]