Multiscale Characterization and Modelling of Polyurethane Foams

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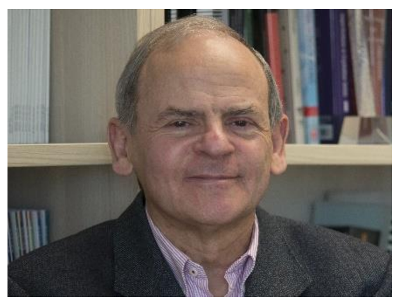

Citations	13517
h-index	64
i10-index	207

Dr. Cláudio Lopes

Citations	1975
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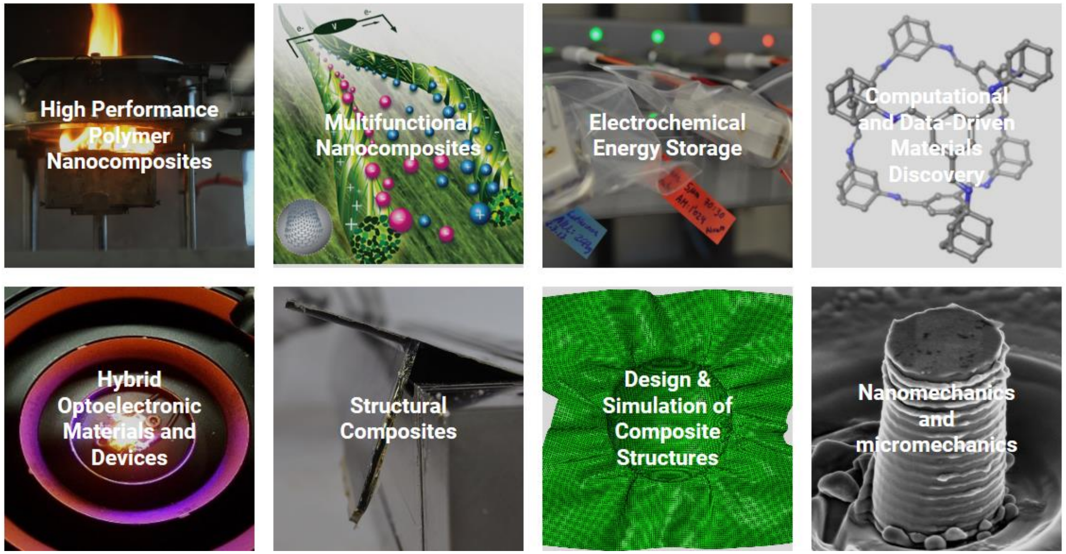
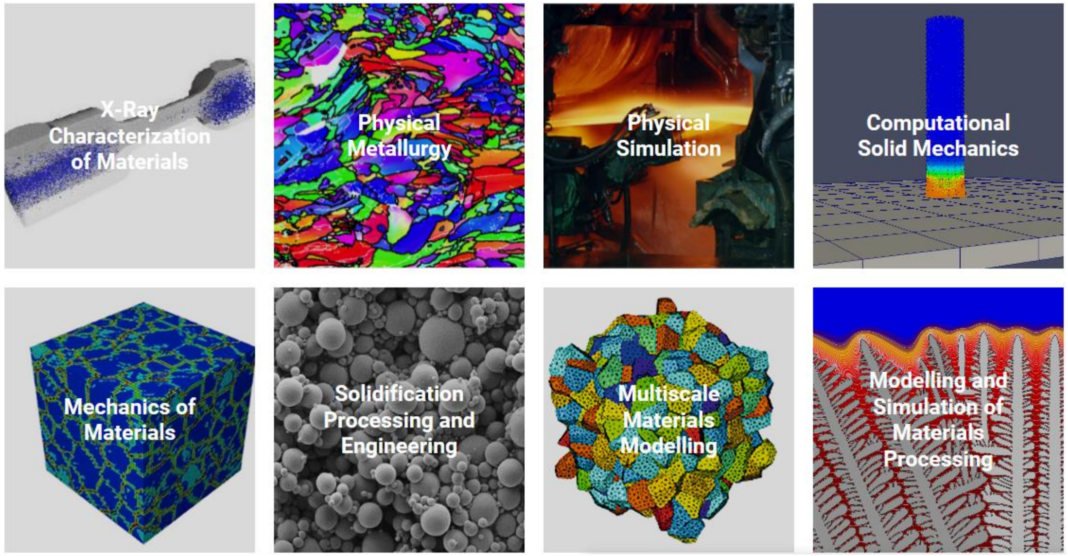
October 14, 2019

Who we are

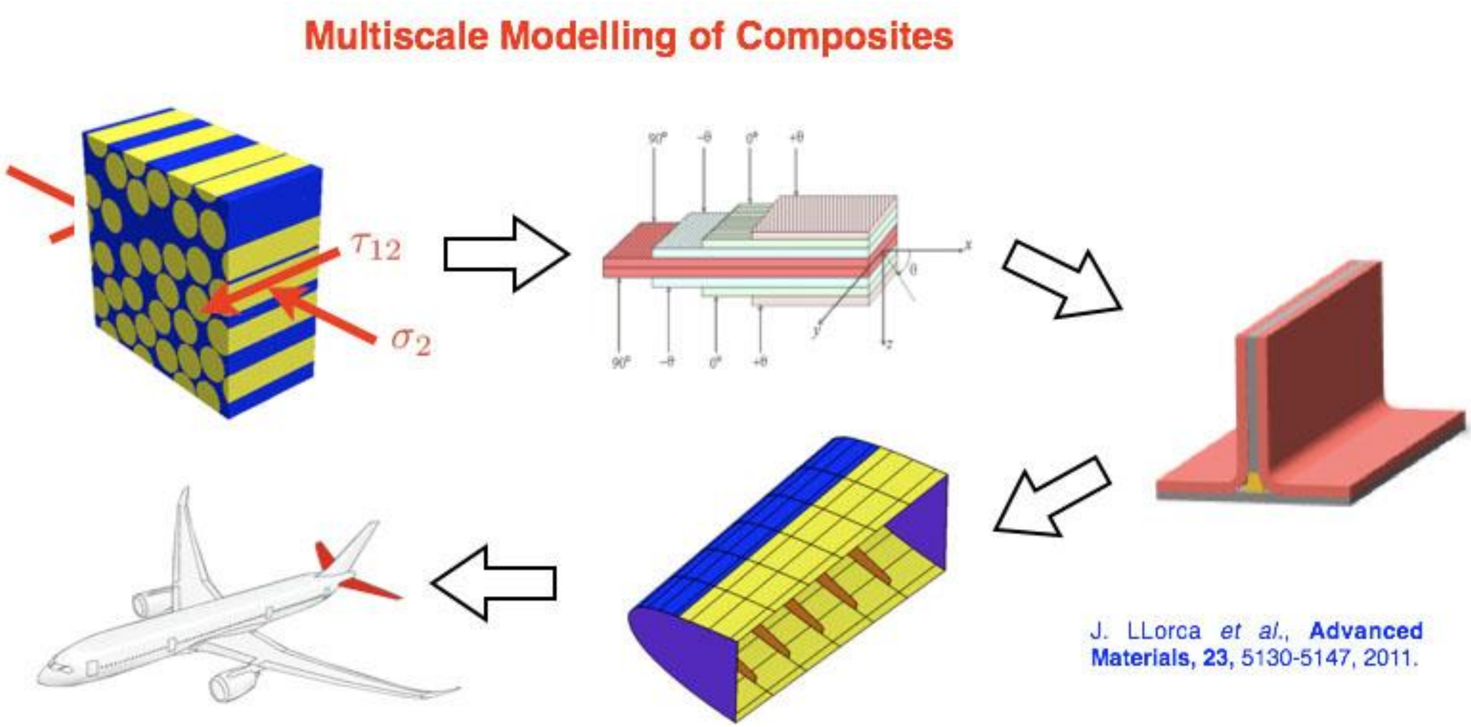


- The IMDEA Materials Institute, one of the seven Madrid Institutes for Advanced Studies (IMDEA), is a public research centre founded in 2007.
- 16 research groups.
- Over 150 people do research at the Institute, including more than 45 post-doctoral scientists and 60 pre-doctoral students.
- currently publishing above 120 JCR journal articles per year.
- more than 70 industrial projects.



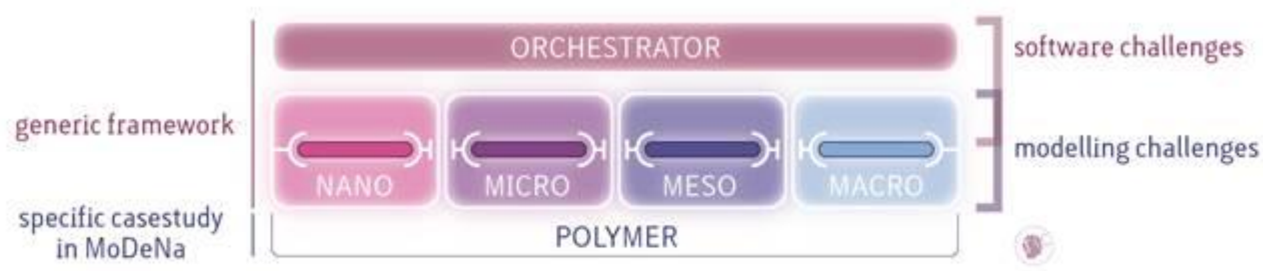
Multiscale modelling of materials

- **Virtual design of materials.**
- **Lets link different scales to optimize the design.**



MOdelling of morphology DEvelopment of micro- and NAnostructures (MoDeNa)

- MoDeNa focuses on the development of an easy-to-use **multi-scale software-modelling framework application** under an **open-source licensing scheme** that delivers models with feasible computational loads for process and product design of complex materials.



Contents

Polyurethane (PU) foams

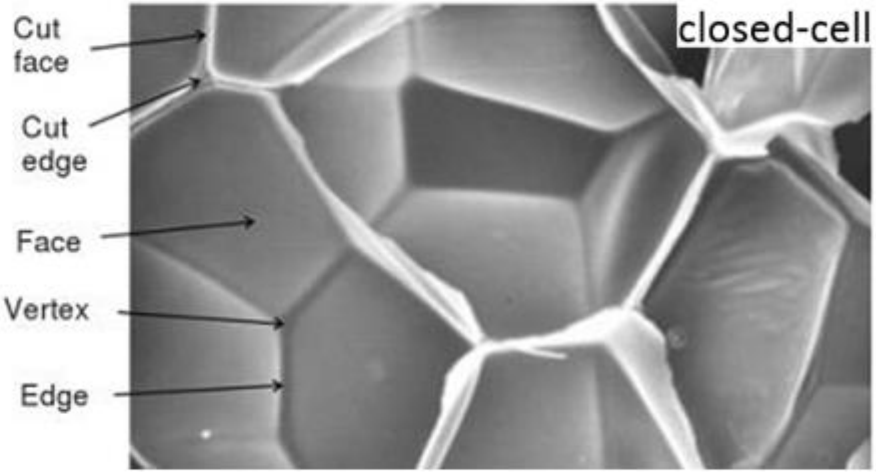
Polyisocyanates + Polyol = Polyurethane + Blowing agent (e.g. CO_2)

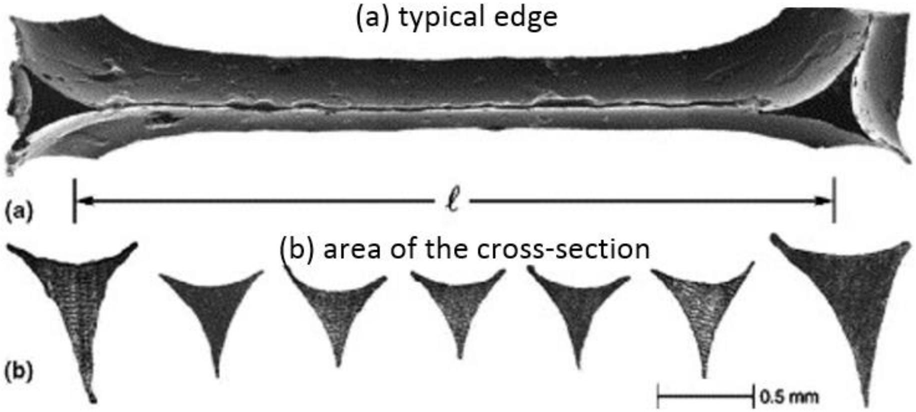
- Polyurethane foams are used in many engineering applications due to their unique combination of properties (low density, high acoustic isolation, large elastic deformability, excellent energy absorption under impact, etc.)

  - impact-friendly surfaces (e.g. automobile interiors)
  - packaging material
  - lightweight composite structure components
  - …

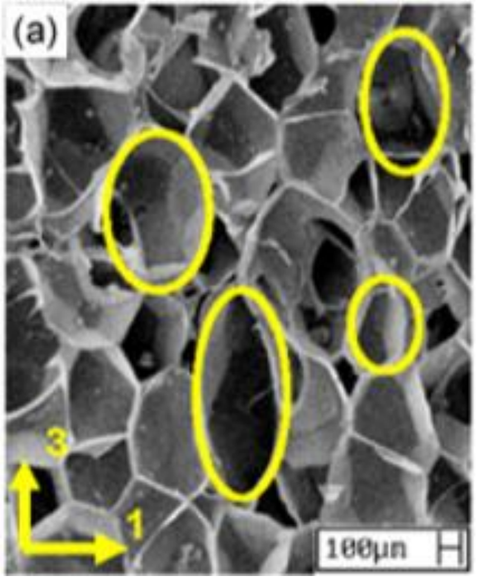
- Global polyurethane foam market: 9.46 million tons in 2015
  12.74 million tons by 2024 (estimated).

Microstructure of PU foams



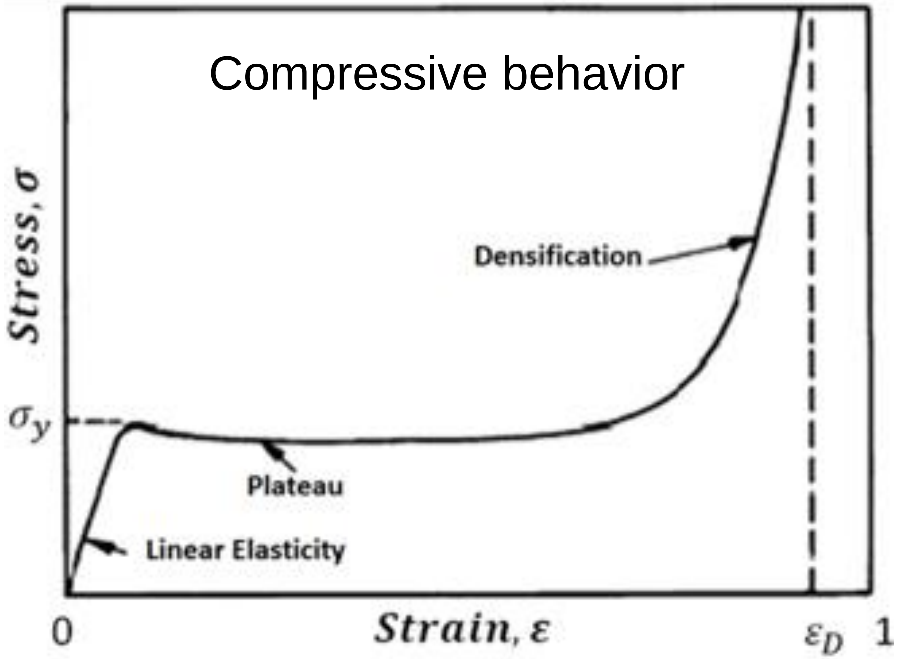


- Cell size distribution
- Anisotropy
- Solid PU distribution between faces (wall thickness) and struts
- Solid PU distribution along the struts
- Fraction of open cells in a close-cell foam



The microstructure of PU foams is very complex and can be tailored to provide very different properties.

Mechanical properties of PU foams



Mechanical behavior of PU foams depend on microstructure

- Linear elastic region (<5%): Bending of struts.
- Plateau region: Cells begin to collapse by elastic buckling, plastic yielding or brittle crushing.
- Densification region: Contact between faces in the cells.

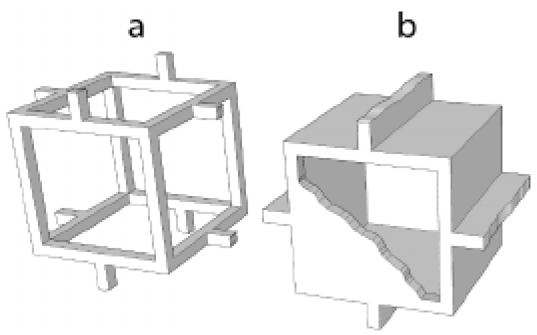
Modelling of mechanical behavior of PU foams

Phenomenological models

- Simple cubic cell model by Gibson and Ashby:

$$\frac{E}{E_s} = c_1 \phi^2 \left(\frac{\rho}{\rho_s}\right)^2 + c_1'(1-\phi)\left(\frac{\rho}{\rho_s}\right)$$

$$\frac{\sigma_y}{\sigma_{ys}} = c_3 \left(\phi \frac{\rho}{\rho_s}\right)^{1.5} + c_4 (1-\phi)\frac{\rho}{\rho_s}$$



Phenomenological models can only provide a approximation to the mechanical properties of foams.

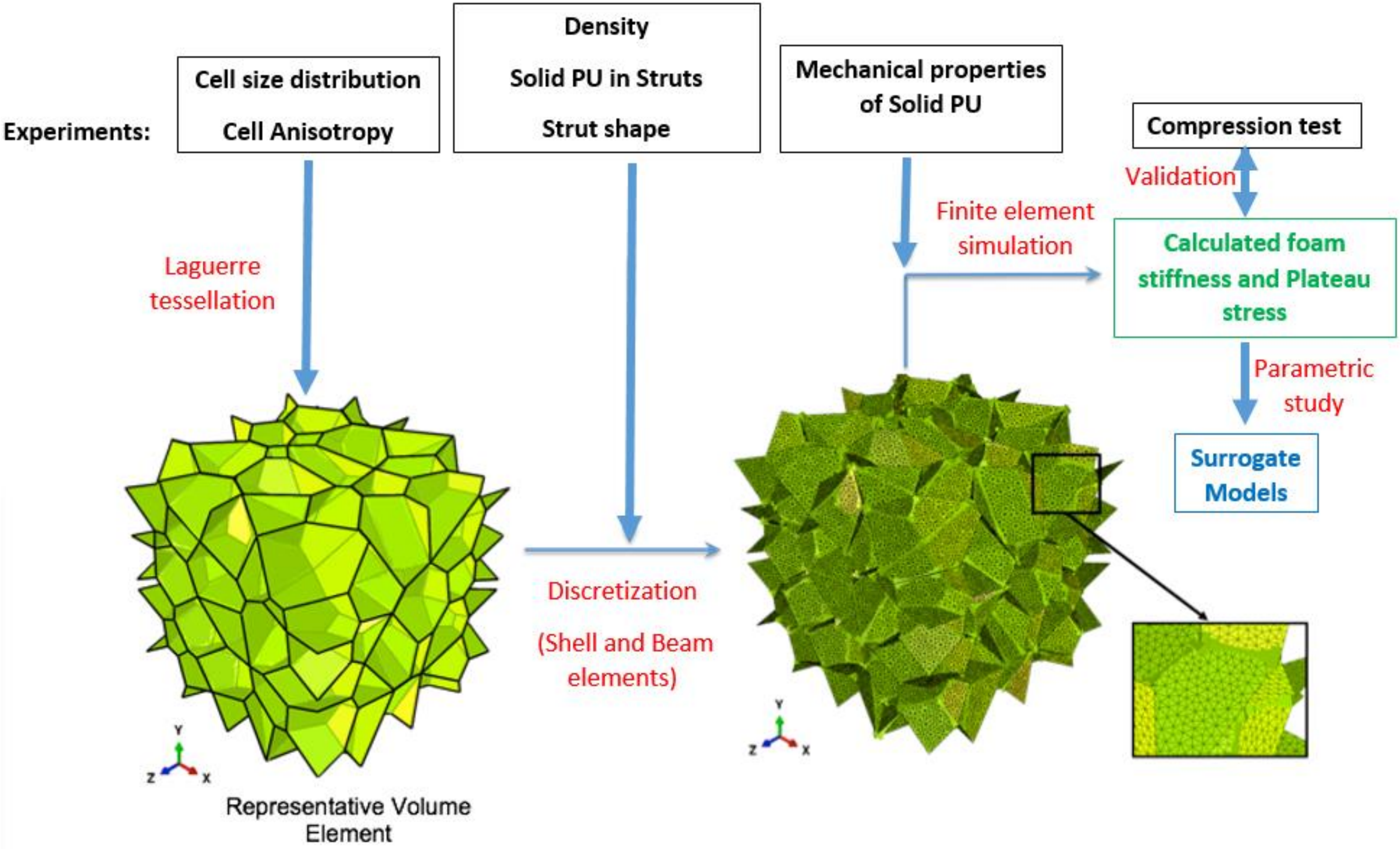
Gibson, L. J., Ashby, 1999. Cellular Solids. Cambridge University Press.

Objectives

- Development of a **comprehensive modeling strategy** able to relate the complex microstructure of the foams with the macroscopic mechanical properties.

- Development of **surrogate models** that can estimate the main mechanical properties (elastic modulus and plateau stress) of closed-cell and open-cell foams taking into account the influence of the relevant microstructural features.

MULTISCALE SIMULATION STRATEGY



M. Marvi-Mashhadiphic, C. S. Lopes, J. LLorca, "Modelling of the mechanical behavior of the polyurethane foams by means of micromechanical characterization and computational homogenization", International Journal of Solids and Structures, 141, 154-166, 2018.

MATERIAL

Four rigid PU foams with isotropic/anisotropic microstructure provided by BASF Polyurethanes GmbH.

	1-3CPW30	ACPW50
	Isotropic	Anisotropic
Density (Kg/m³)	30±0.2	50±0.6

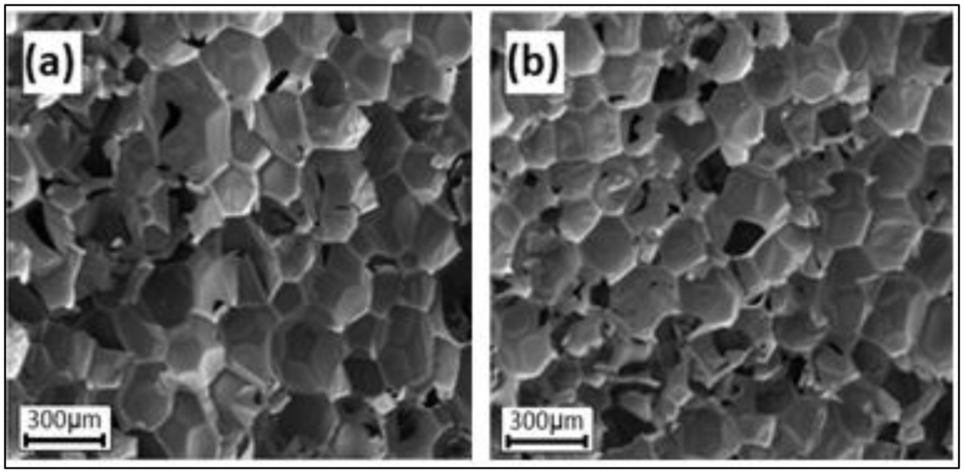
CHARACTERIZATION TECHNIQUES

- Microstructural characterization:
  - Scanning electron microscopy: Cell shape as well as cell wall thickness.
  - X-ray computed tomography: Cell size distribution and strut shape.
- Micromechanical characterization:
  - Instrumented nanoindentation: Viscoelastic properties of the solid PU. Yield strength of the solid PU.
- Mechanical characterization:
  - Mechanical tests (compression): Macroscopic mechanical properties.

FOAM MICROSTRUCTURE

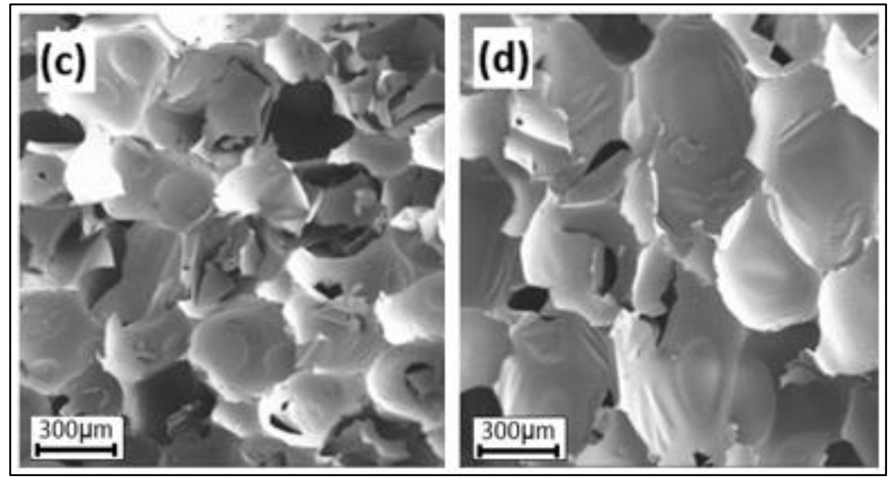
Cell shape

1-3CPW30 (Perpendicular) | 1-3CPW30 (Parallel)



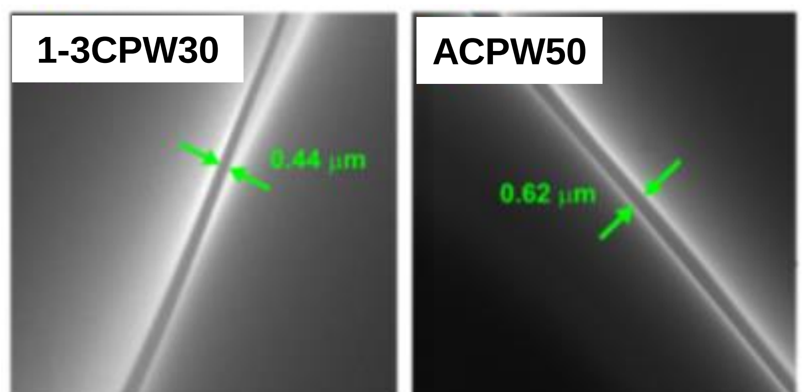
Aspect ratio ≈ 1

ACPW50 (Perpendicular) | ACPW50 (Parallel)



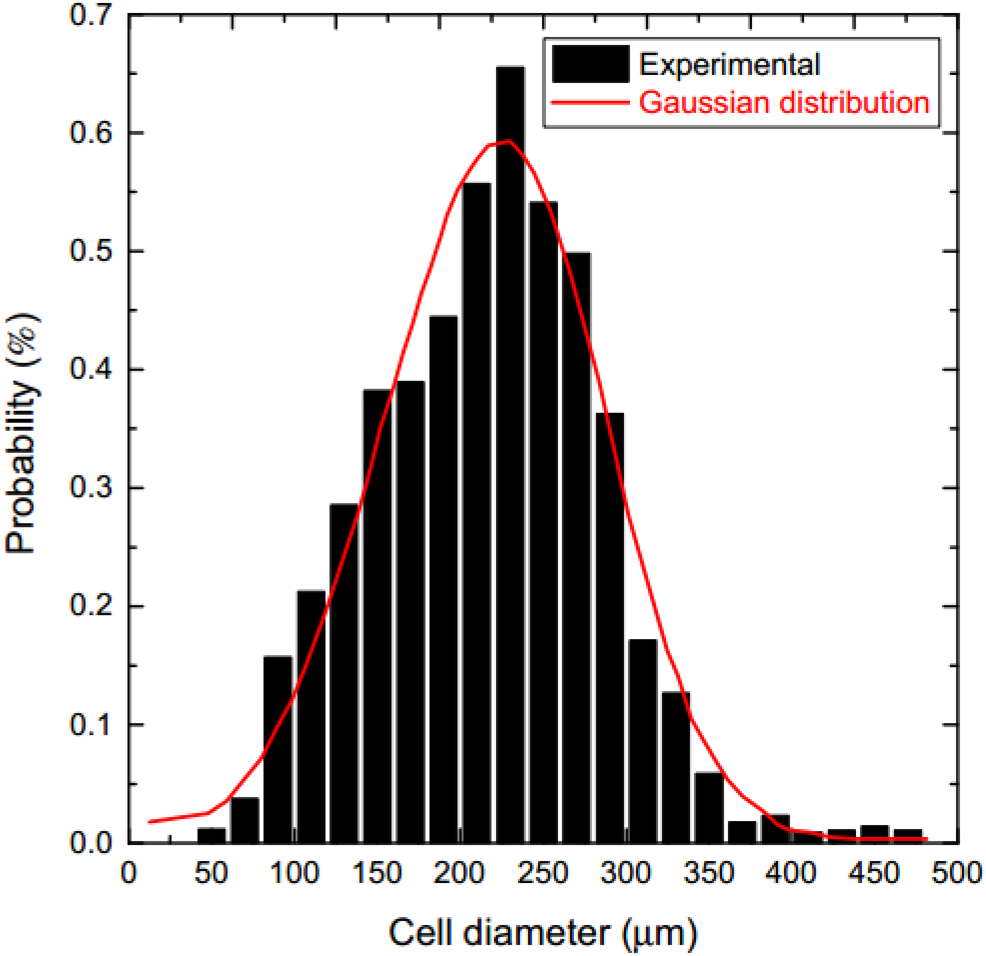
Aspect ratio = 1.3 ± 0.04

Cell wall thickness



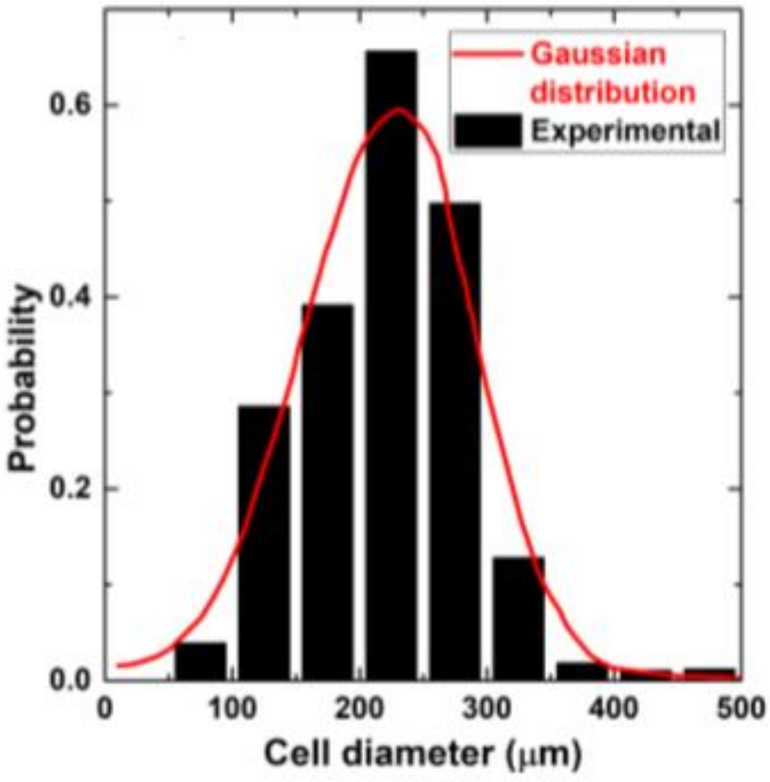
CELL SIZE DISTRIBUTION

Cell size distribution of the PU foam measured by XCT and Gaussian cell size distribution used in the simulations.

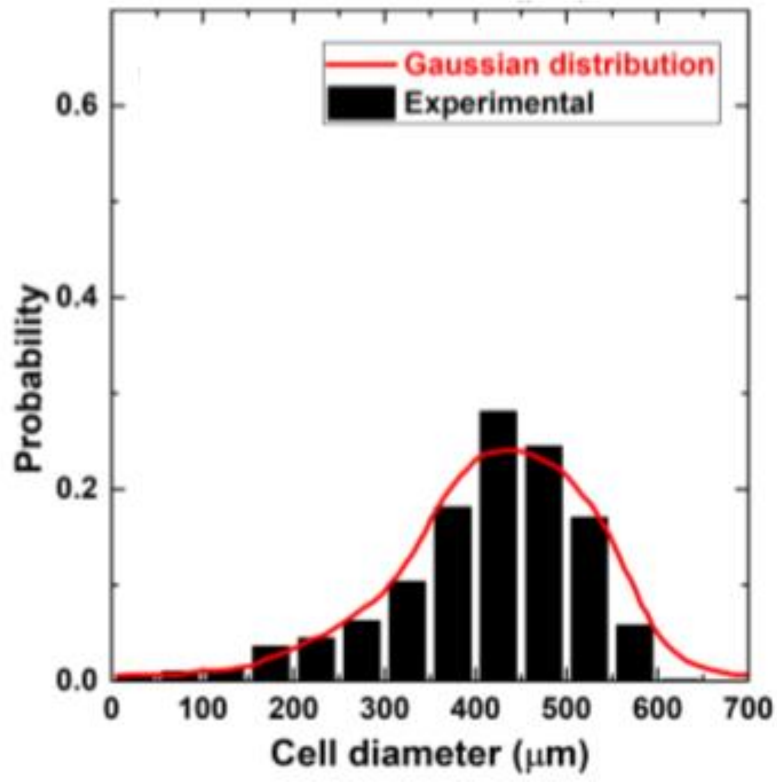


CELL SIZE DISTRIBUTION

1-3CPW30



ACPW50

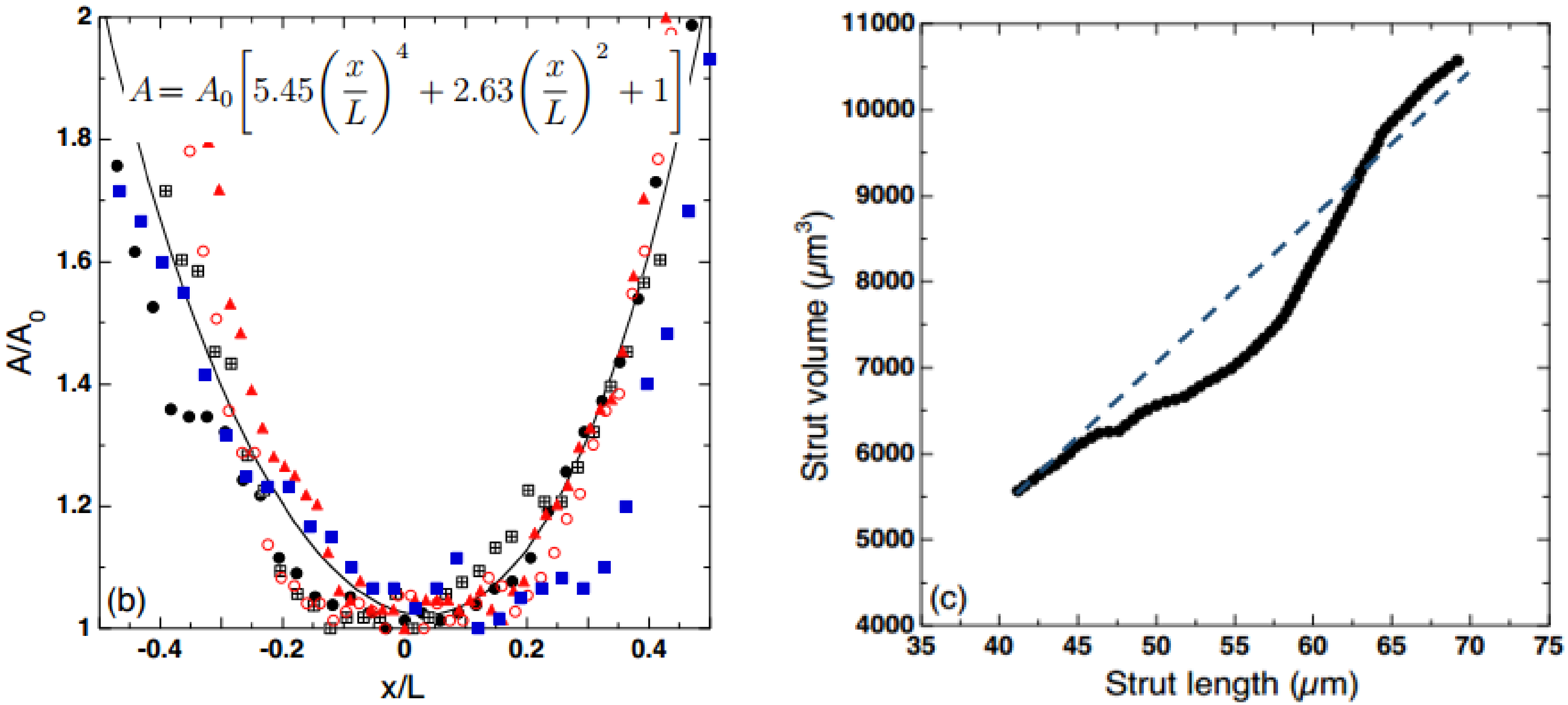


Cell size distribution follows the Gaussian distribution.

Nistor A., Toulec M., Zubov A. & Kosek J. (2016). Tomographic reconstruction and morphological analysis of rigid polyurethane foams. Macromolecular Symposia, 360, 87–95.

STRUT SHAPE

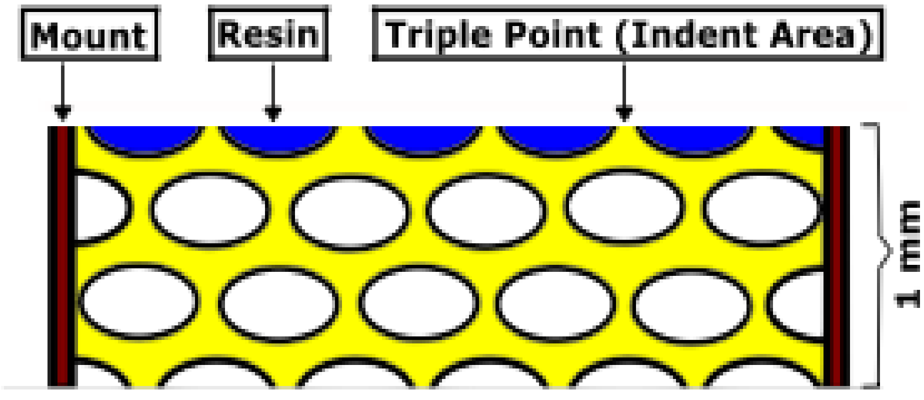
X-ray tomography



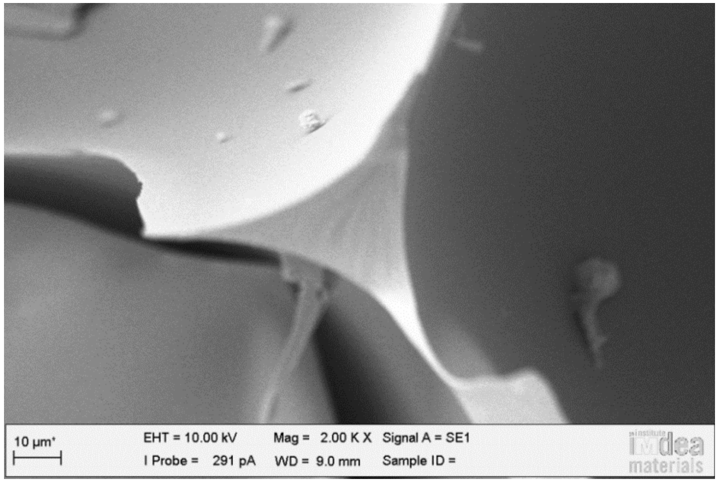
Strut volume is approximately proportional to the length.

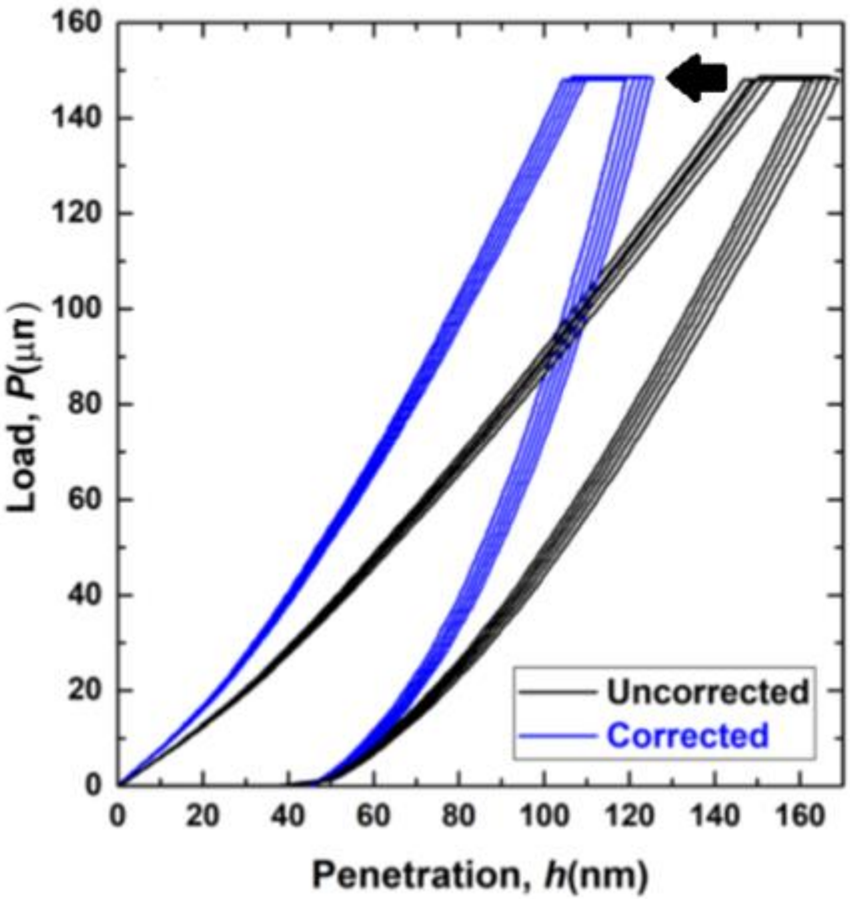
VISCOELASTIC PROPERTIES OF THE SOLID PU

- Viscoelastic properties of solid PU were obtained by means of spherical nanoindentation creep test.
- The mayor problem to carry out nanoindentation in cellular solids is the additional compliance due to pores.



Nanoindentation sample





Spherical indentation

Elastic

$$h^{3/2} = \frac{3}{8\sqrt{R}}\left[\frac{P}{2G}\right]$$

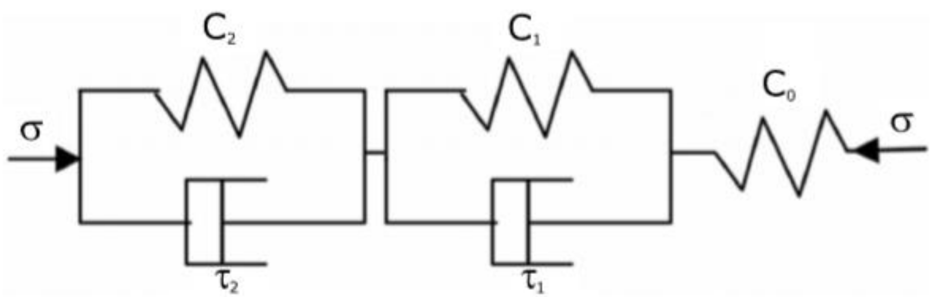
Replacing [P/2G] with viscoelastic integral

Viscoelastic

$$h^{\frac{3}{2}}(t) = \frac{3}{8\sqrt{R}}\int_0^t J(t-u)\frac{dP}{du}du$$

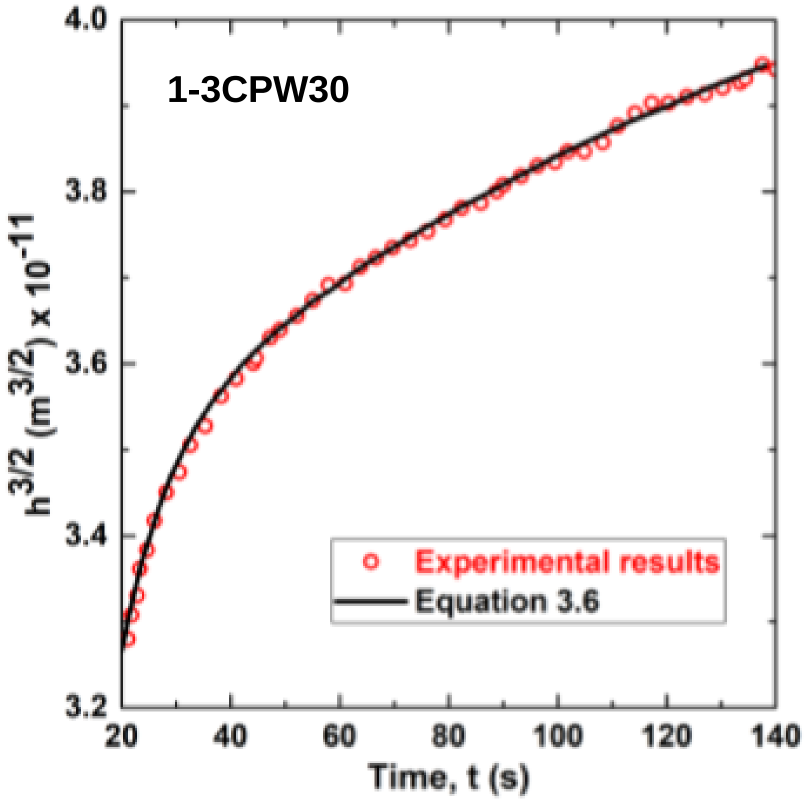
The standard linear viscoelastic solid model used as a material creep function to solve this integral:

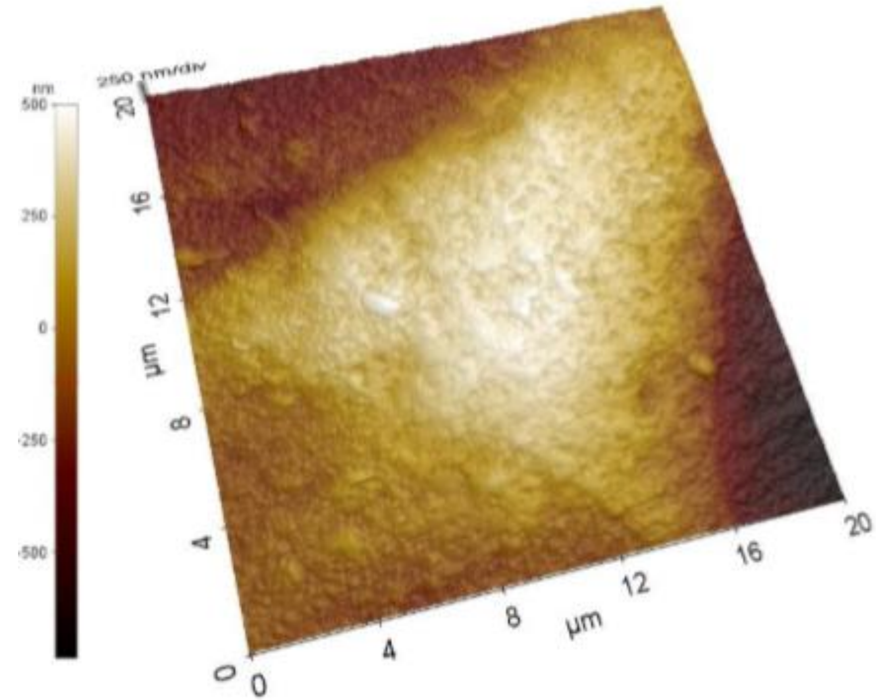
$$J(t) = C_0 - C_1 \exp\left(-\frac{t}{\tau_1}\right) - C_2 \exp\left(-\frac{t}{\tau_2}\right)$$



Johnson K.L. (1985). Contact Mechanics: Cambridge University Press, Cambridge.

VISCOELASTIC PROPERTIES OF THE SOLID PU



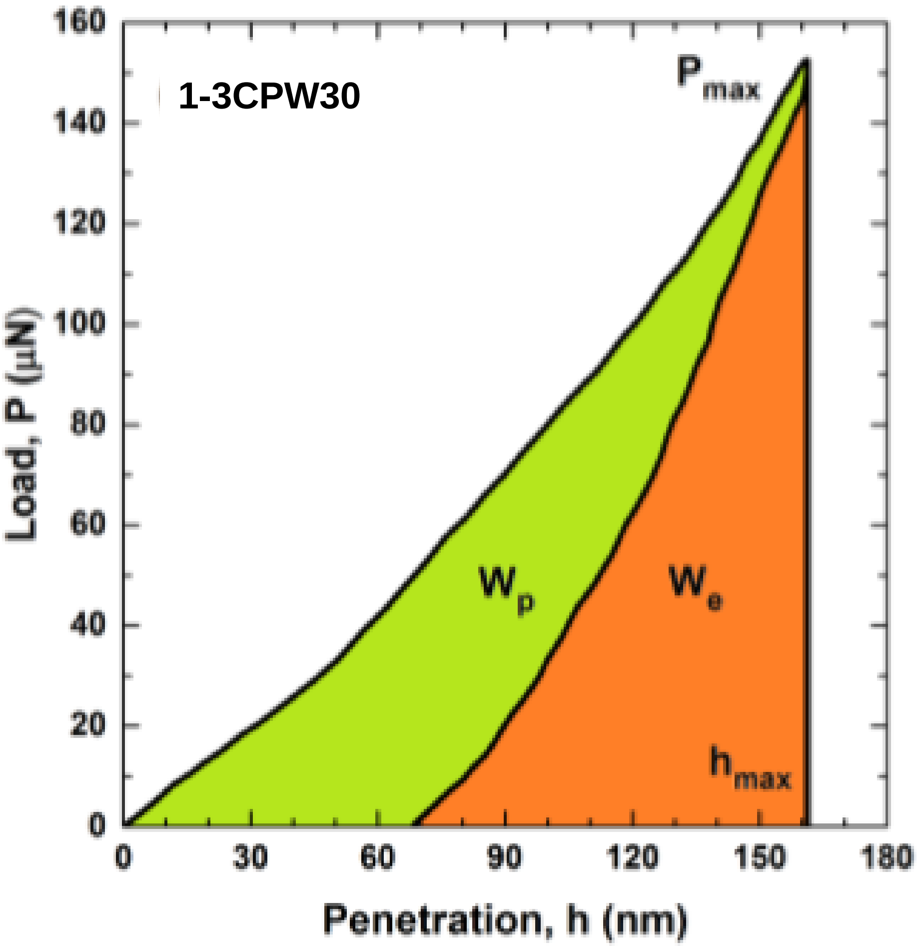


If t=0 : $G = \dfrac{1}{2(C_0 - (C_1 + C_2))} \longrightarrow \begin{cases} E = 2G(1+\vartheta) \\ \vartheta = 0.35 \end{cases}$

	E (GPa)
1-3CPW30	2.4±0.1
ACPW50	2.5±0.1

YIELD STRENGTH OF THE SOLID PU

➢ Yield strength of solid PU was obtained through Berkovich nanoindentation.

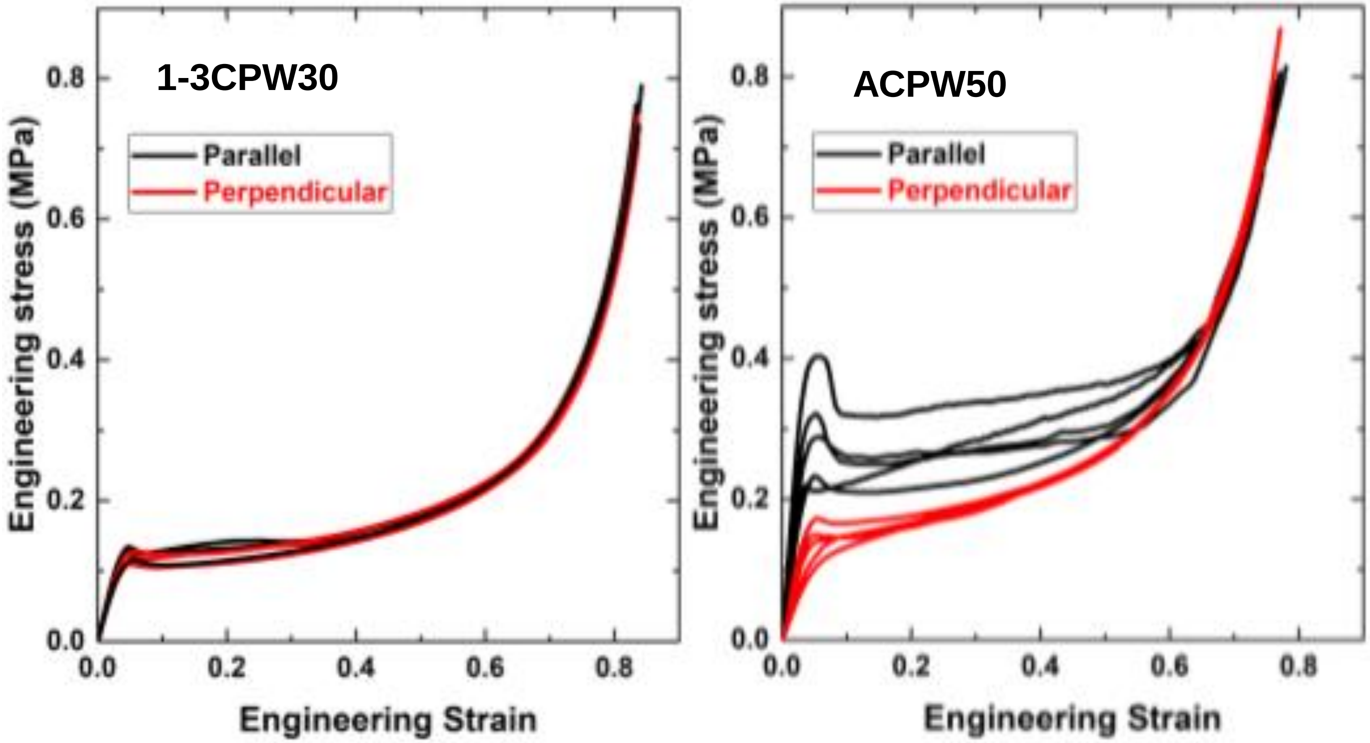


- We/(We + Wp) >0.5, then the Oliver and Pharr method can be used to determine the actual contact area of the tip.
- The compressive flow stress of the PU can be obtained from hardness H using equations and graphs developed by Rodriguez *et al*.

	σ_y (MPa)
1-3CPW30	110 ± 2
ACPW50	109 ± 3

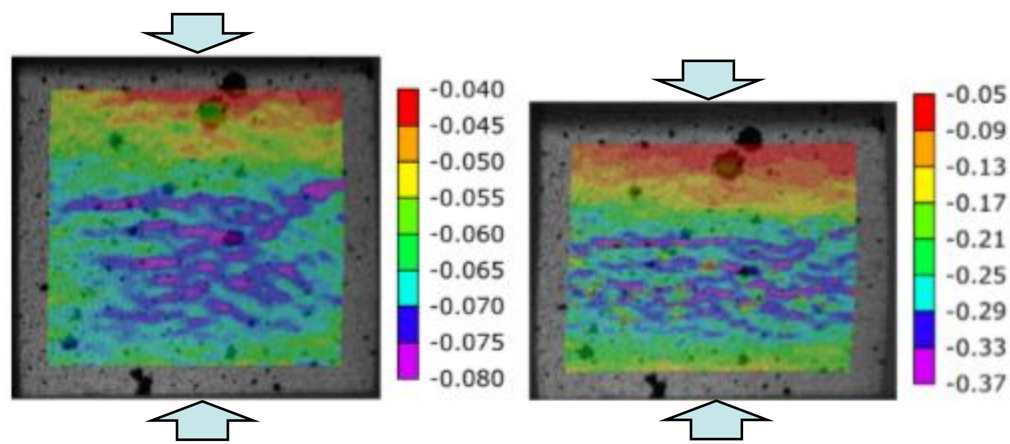
Rodriguez M., Molina-Aldareguıa J.M., Gonzalez C. & LLorca J. (2012). Determination of the mechanical properties of amorphous materials through instrumented nanoindentation. Acta Materialia, 60, 3953 – 3964.

Compressive deformation



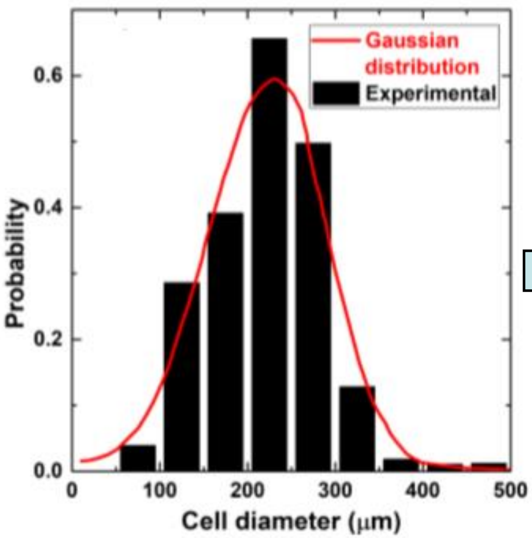
Digital Image Correlation (DIC)

Engineering strain=-7% Engineering strain=-20%

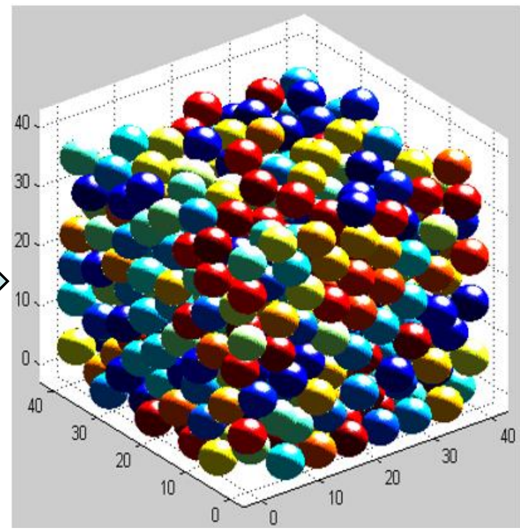


RVE construction

Laguerre tessellation.

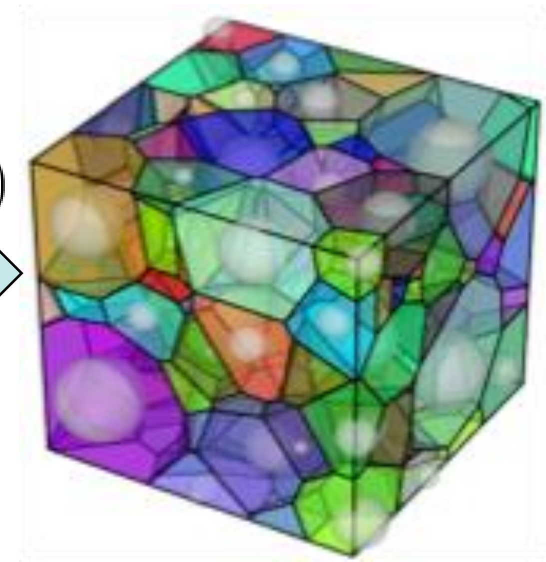


Cell size Distribution



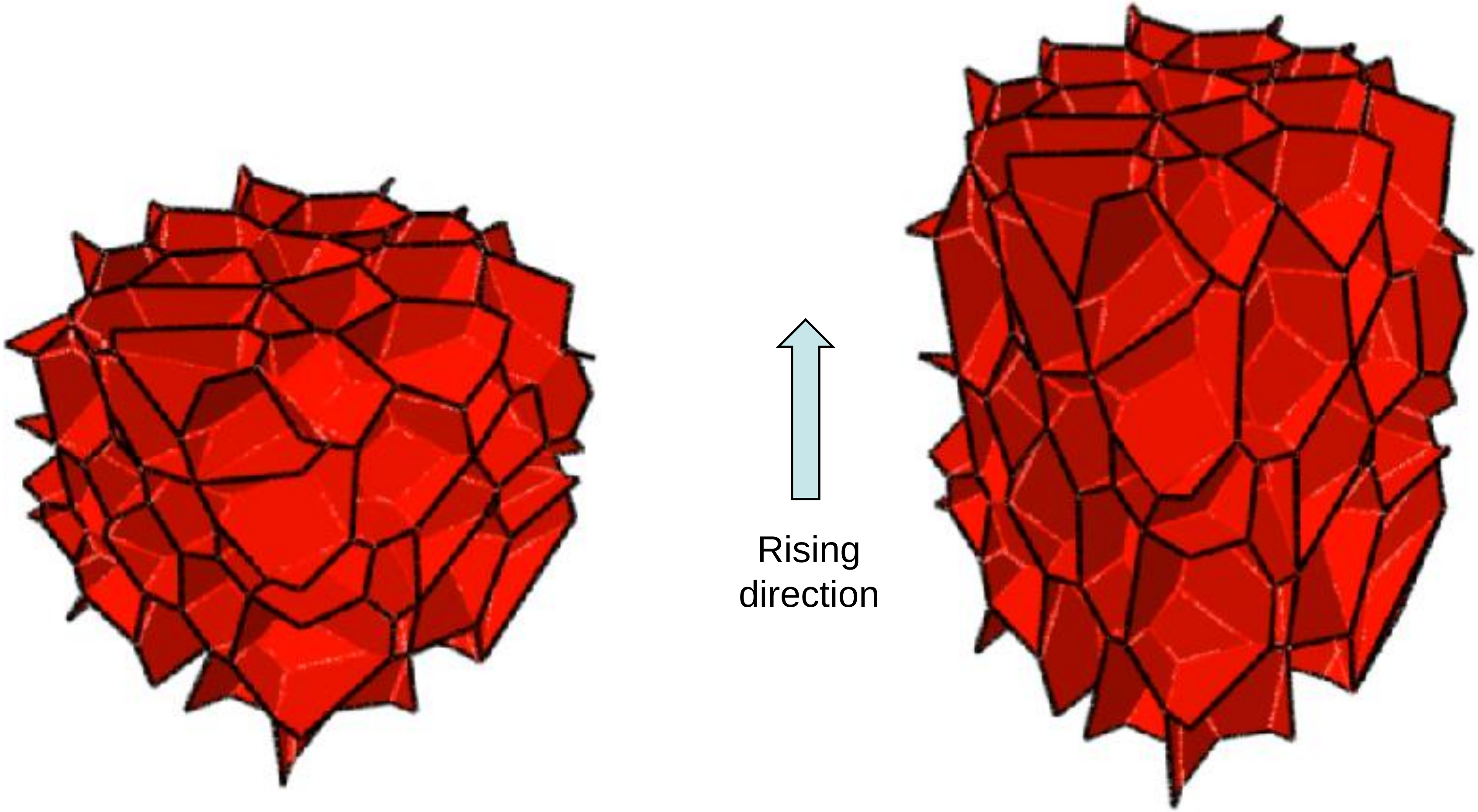
Packing of spheres
(Force biased Algorithm)

$(\mathbf{x}_i, r_i)$



3D Laguerre tessellation
(NEPER)

Foam topology



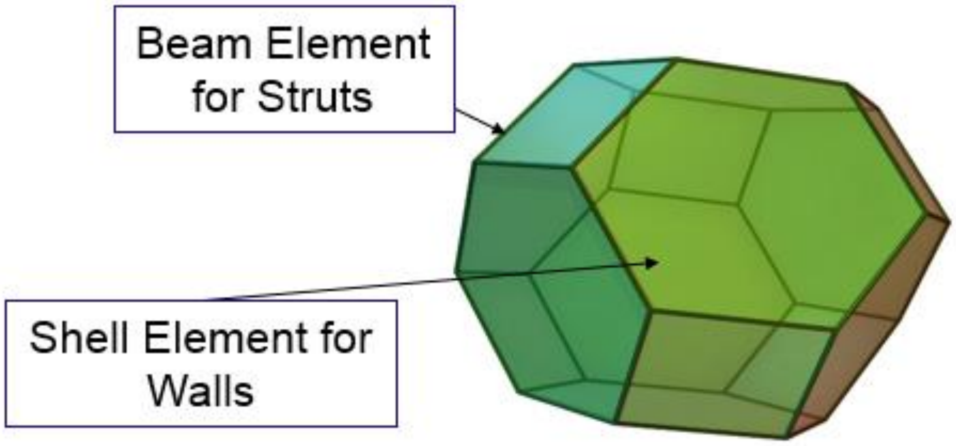
Isotropic **Anisotropic**

Finite element model

- Mass of solid PU in RVE

$$m_{SolidPU} = V_{RVE}\rho_f \Rightarrow V_{SolidPU} = \frac{m_{SolidPU}}{\rho_{Solid\ PU}}$$

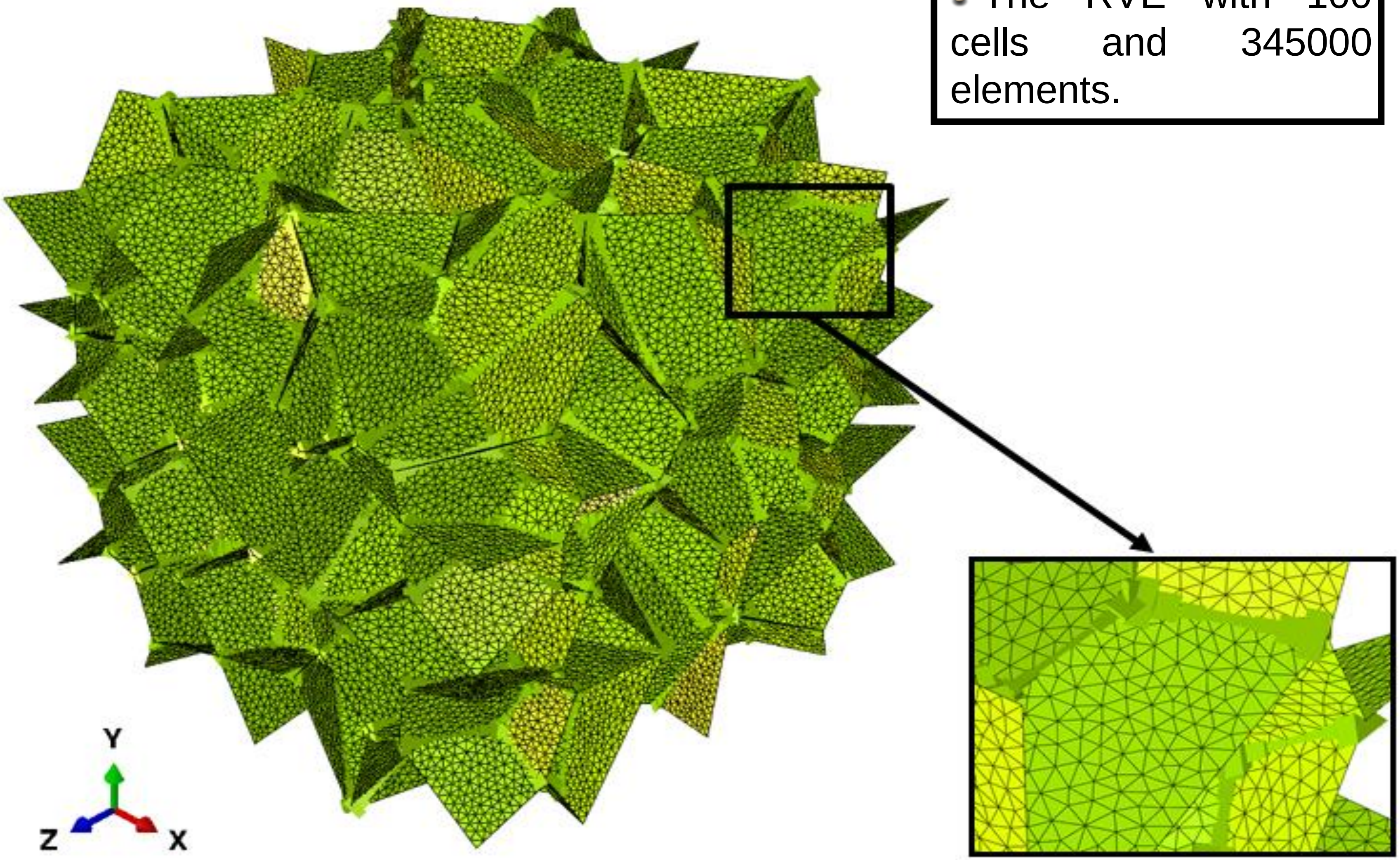
$$V_{SolidPU} = V_{walls} + V_{struts}$$



- The cell wall thickness was constant: $t = \frac{V_{walls}}{\text{Total area of cell faces}}$
- For the strut i: $V_i = \frac{V_{struts} L_i}{L_{struts}}$
- V_i is distributed along the strut i: $A = A_0 \left[5.45 \left(\frac{X}{L}\right)^4 + 2.63 \left(\frac{X}{L}\right)^2 + 1\right]$

Finite element model

- The RVE with 100 cells and 345000 elements.

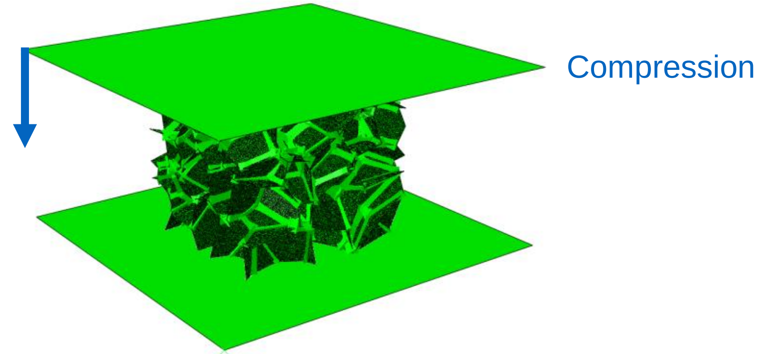


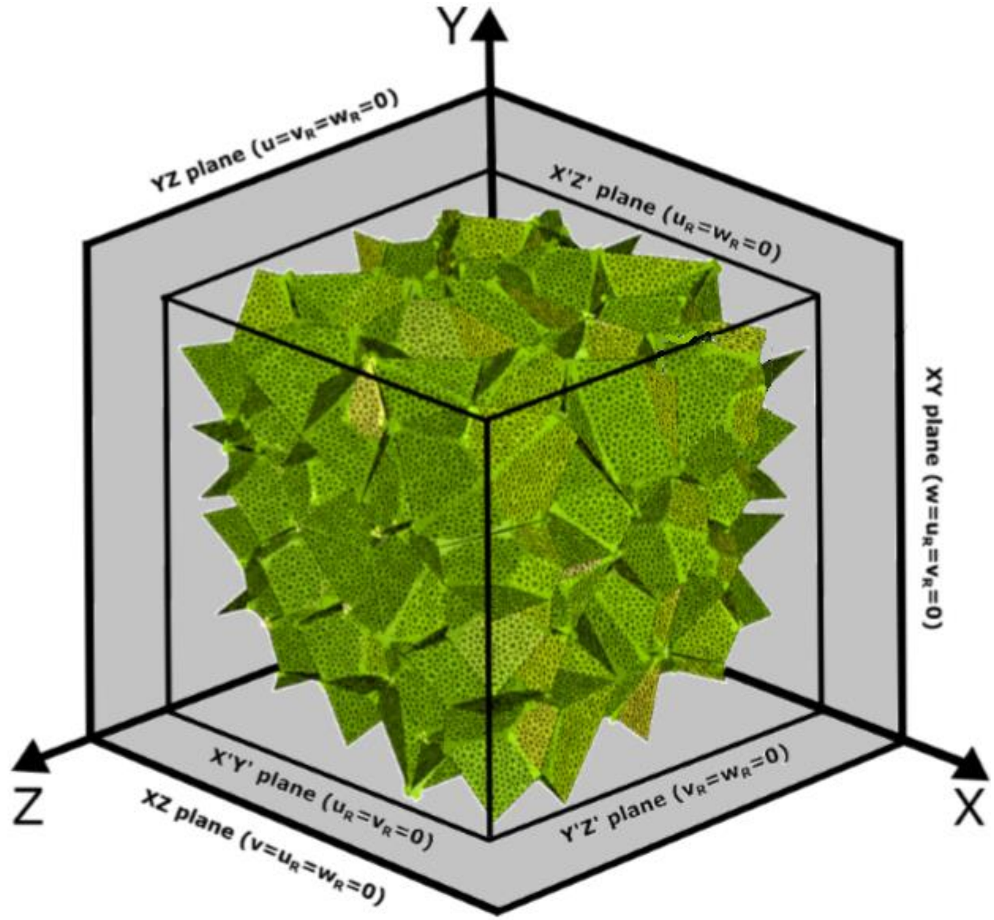
FINITE ELEMENT SIMULATIONS

- The mechanical response of the RVE in compression was obtained by the finite element analysis of the RVE (Abaqus/standard and Abaqus/explicit).

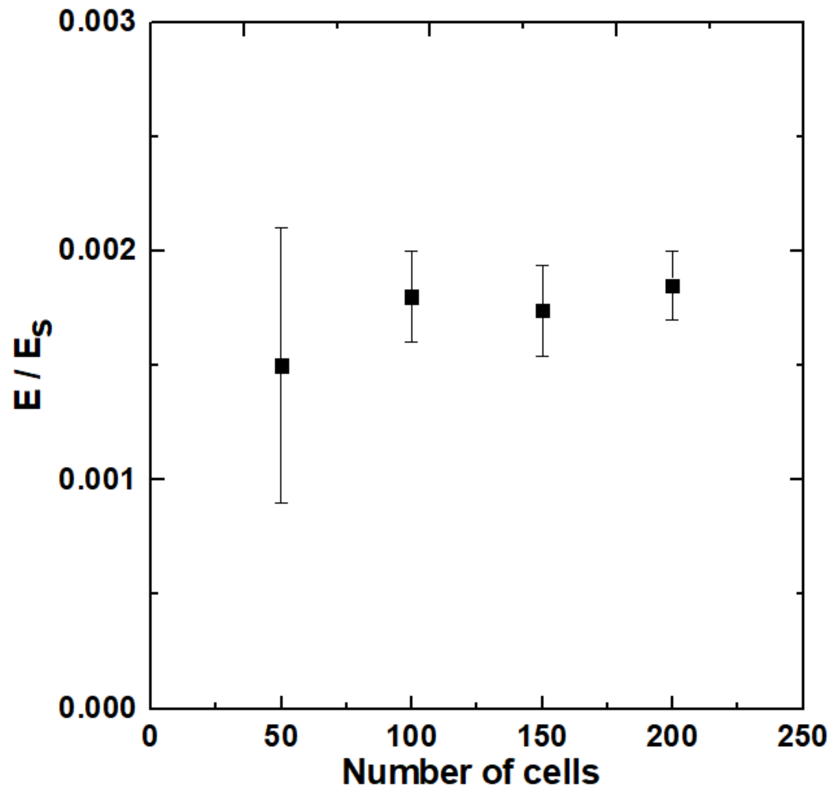
- Compression load was applied by the movement of **two rigid surfaces** in contact with the RVE.

- The solid PU was assumed to behave as an isotropic, elasto-plastic solid.





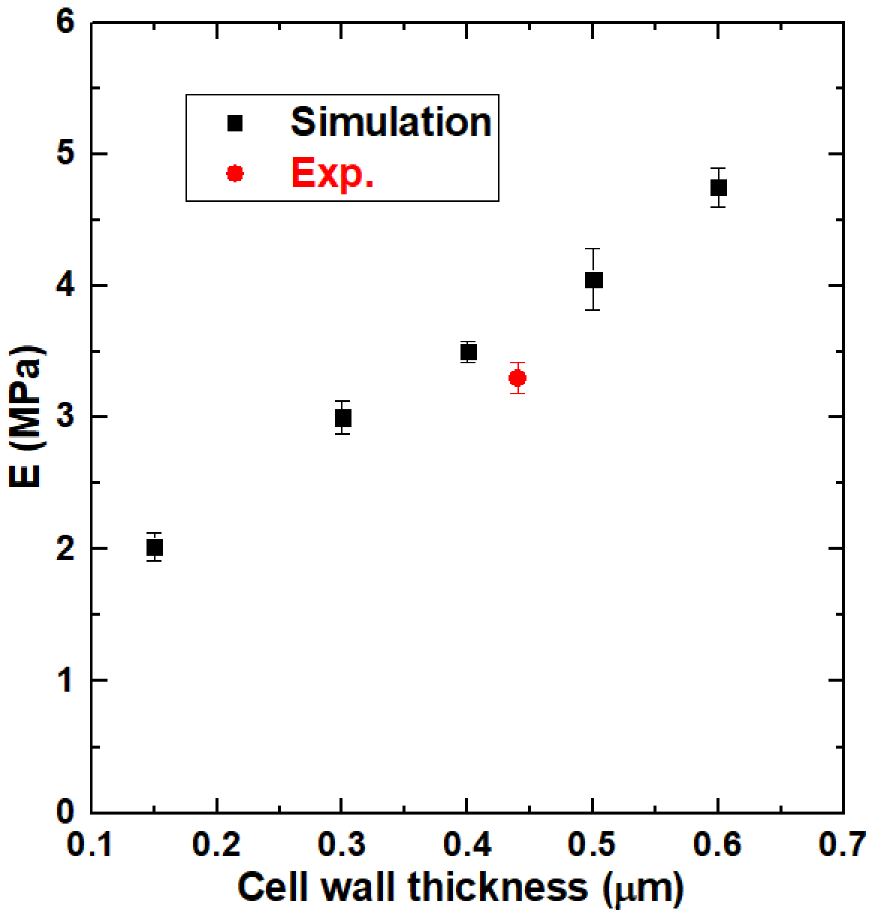
Convergence analysis



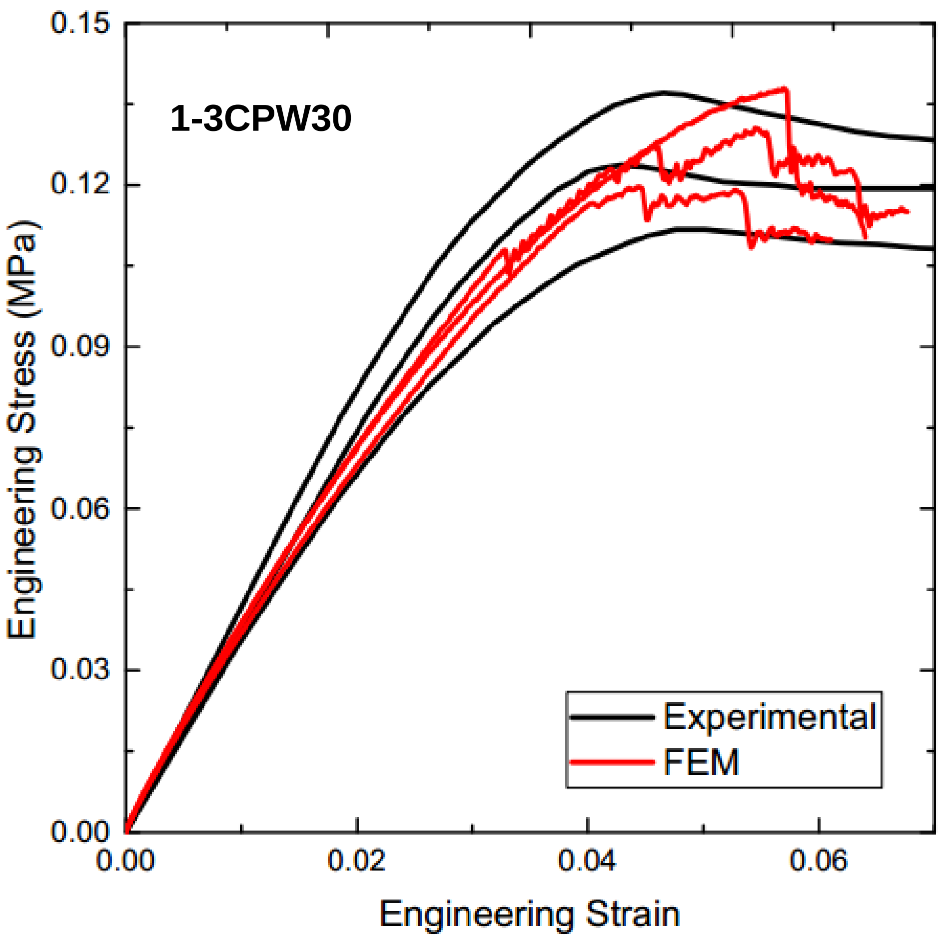
- RVEs with 100 cells were used in the numerical simulations.
- Mesh-independent results was obtained when an average strut was discretized with 21-22 beam elements.

EXPERIMENTAL VALIDATION

Elastic modulus



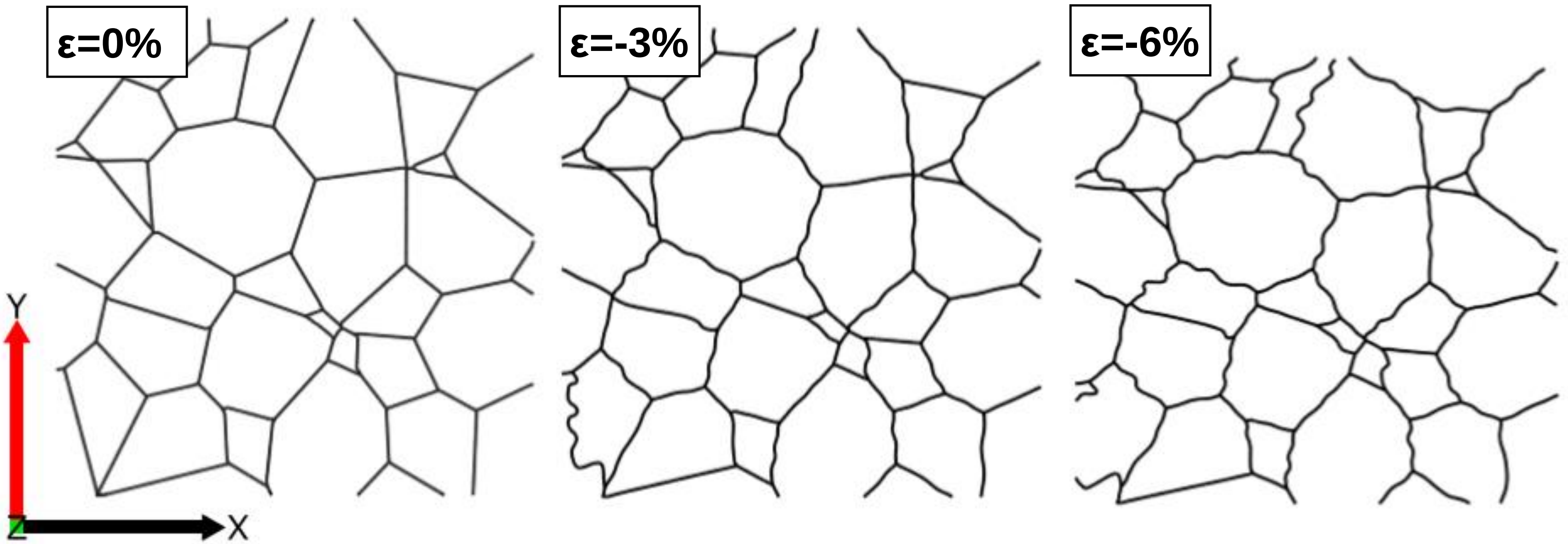
Plateau stress



The multiscale modelling strategy was able to predict the foam elastic modulus and Plateau stress.

Deformation Mechanisms

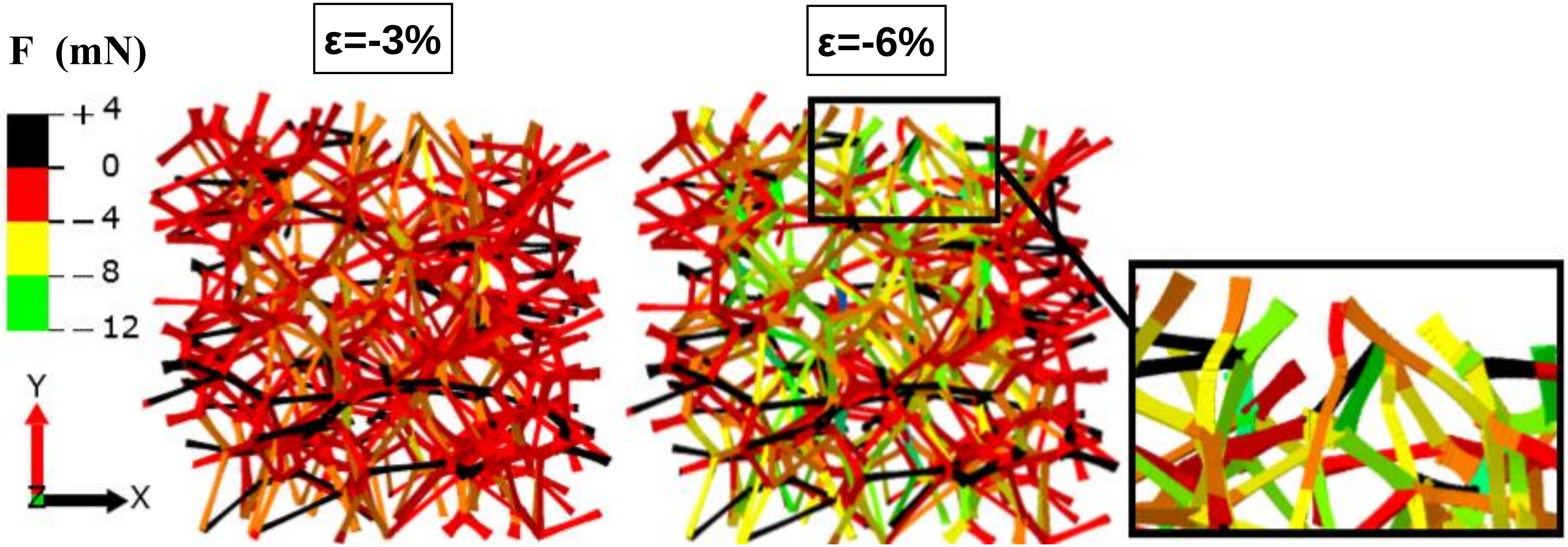
Cross-sections of the foam microstructure at different compressive strains.



- Buckling of the cells faces occurs very early (ripples in the cell walls).
- Cell wall buckling was not responsible for the plateau region and localization of damage.

Deformation mechanisms

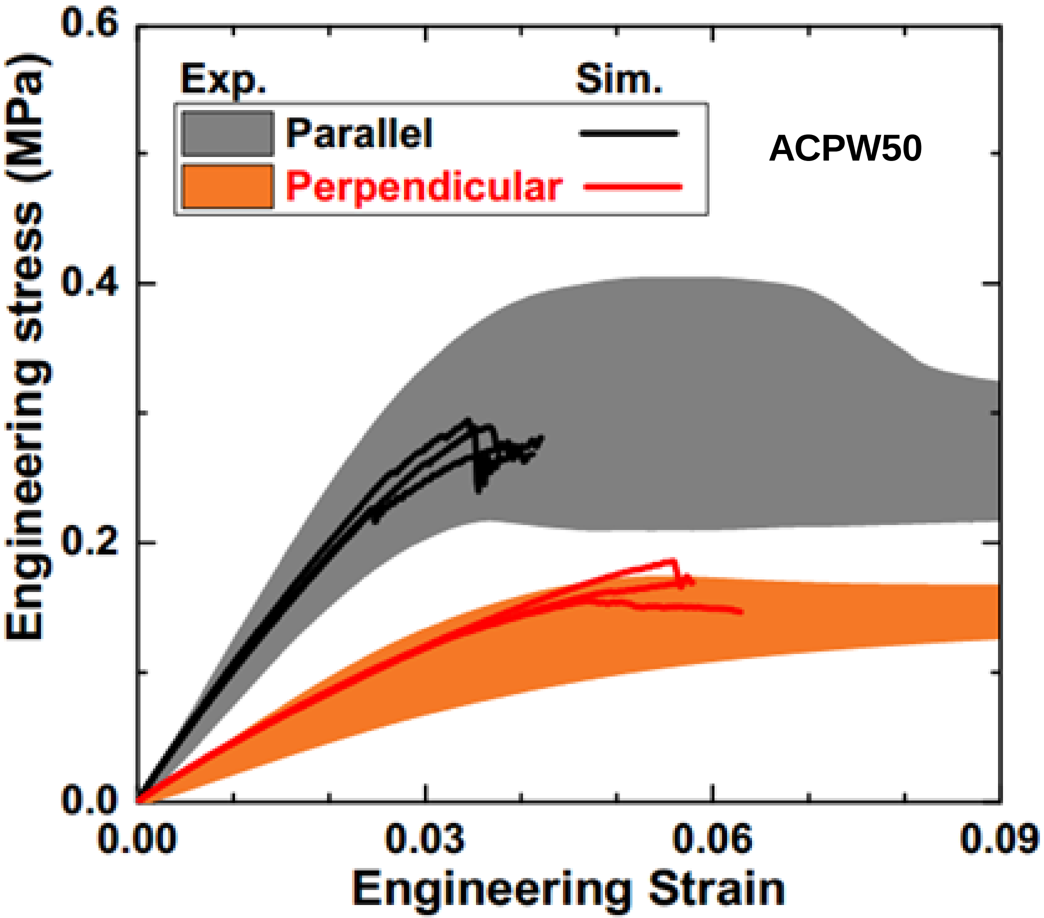
Contour plot of the axial force in the strut network.



- The load in the elastic regime is homogeneously distributed at 3% strain.

- The struts located at the top after 6% strain have buckled in response to the high compressive load along their axis.

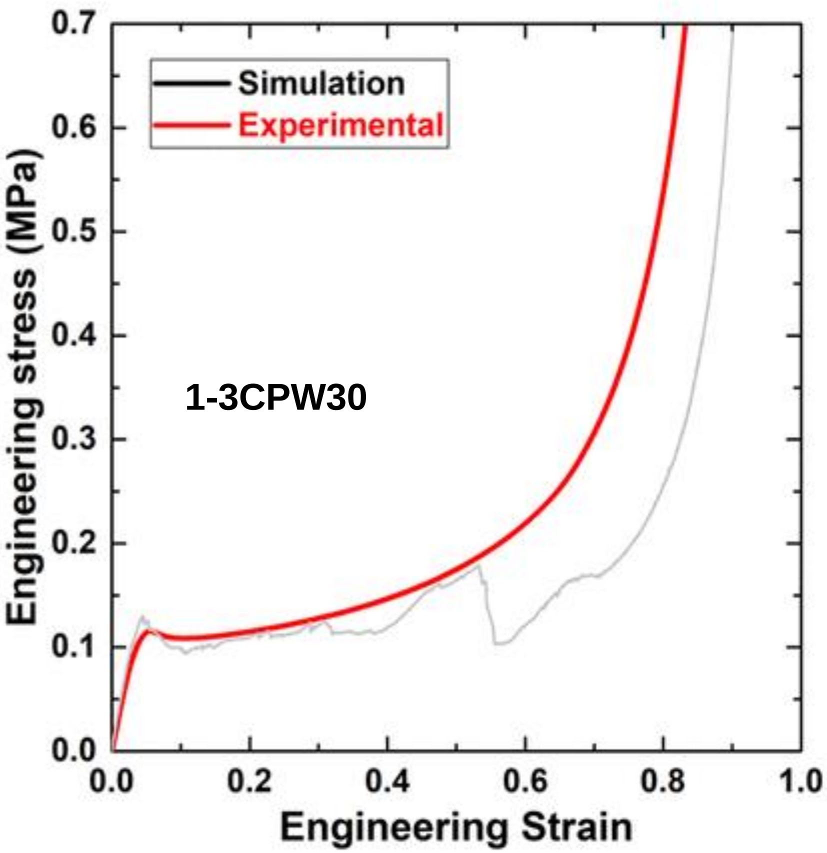
EXPERIMENTAL VALIDATION

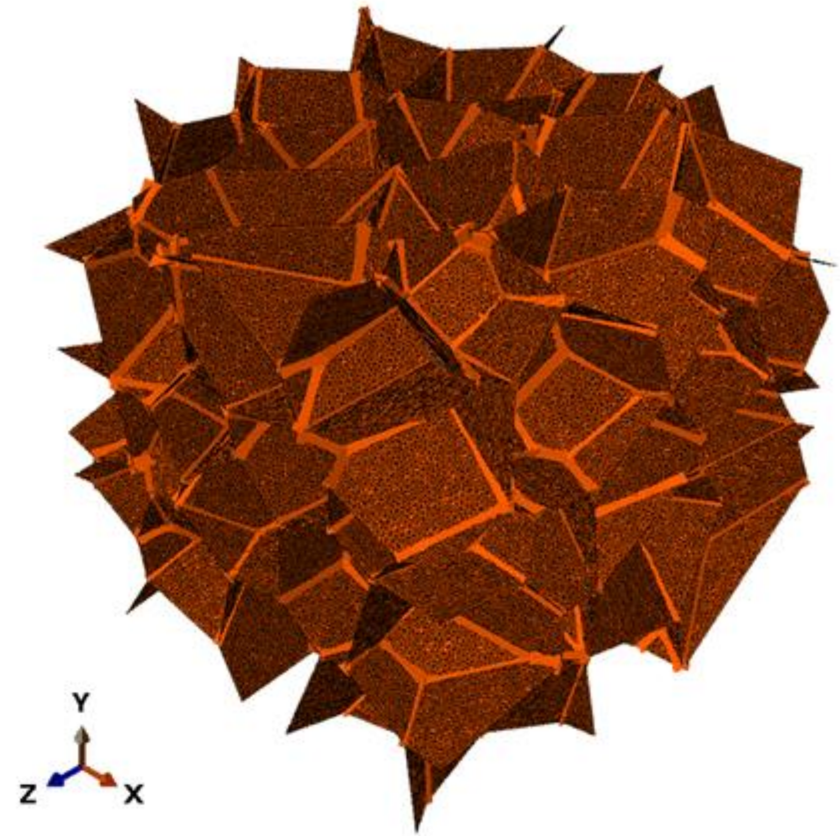


- Modelling strategy is able to capture the strong effect of anisotropy on the elastic modulus and Plateau stress.

M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, " Effect of anisotropy on the mechanical properties of polyurethane foams: an experimental and numerical study", Mechanics of Materials, 124, 143-154, 2018.

Numerical simulation up to densification

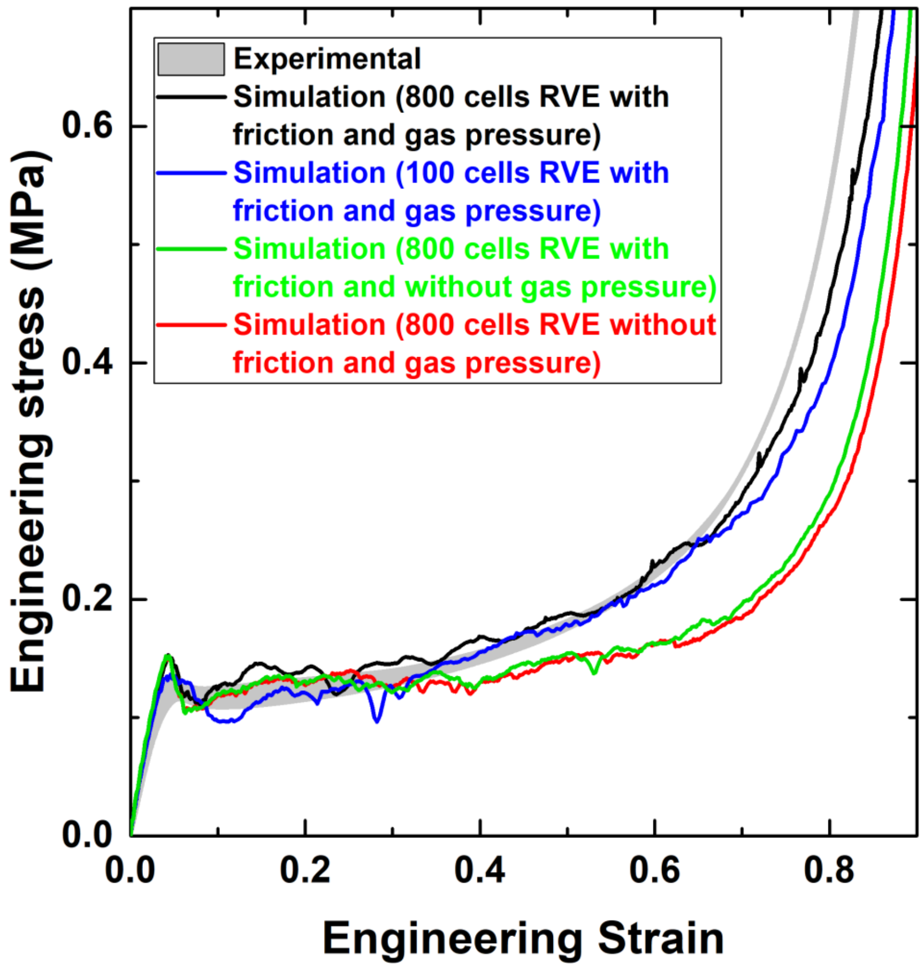




- Simulations were carried out using general contact algorithm and assuming zero friction.
- Internal pressure was not included and might be the reason for postpone in densification.

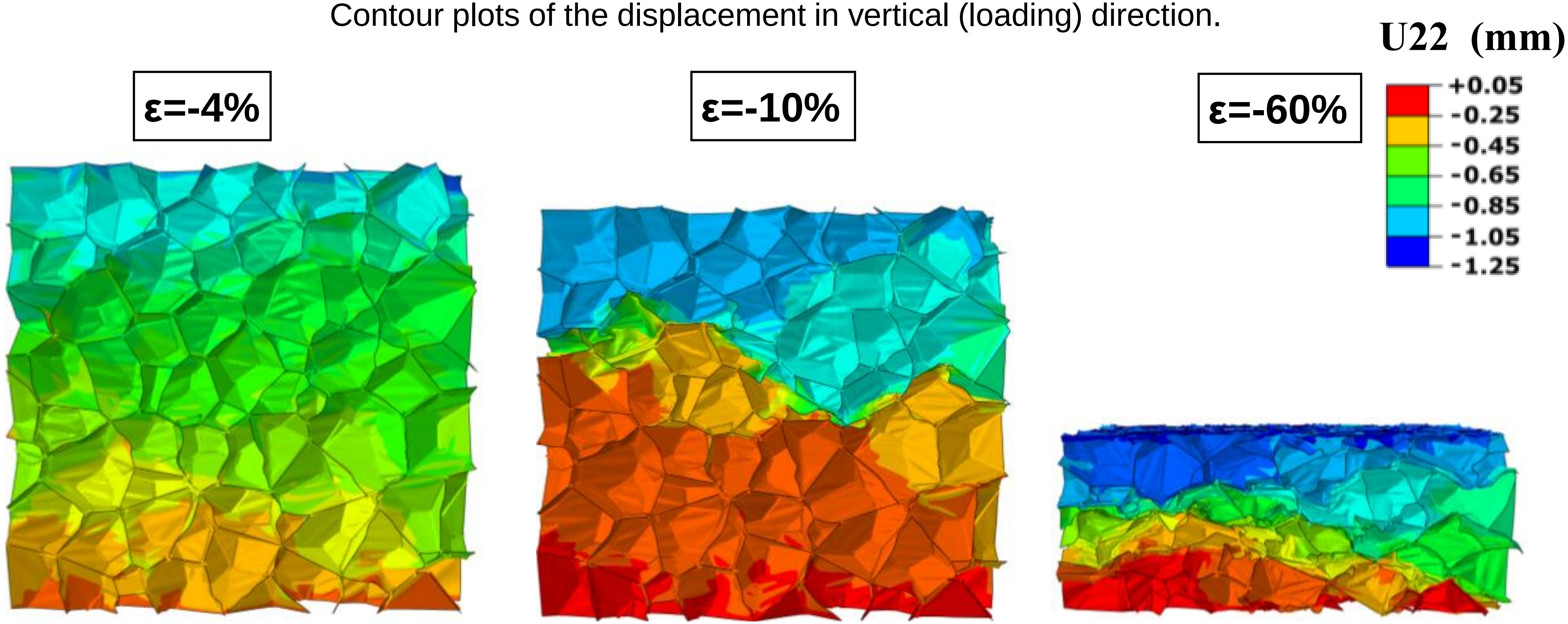
Numerical simulation up to densification

RVE containing 800 cells.



Numerical simulation up to densification

Contour plots of the displacement in vertical (loading) direction.



- A homogeneous distribution of buckled cell walls at 4% strain.

- The gradual increase of the load leads to the progressive collapse of the layers of cells adjacent to the initial collapsed layer until all cells become crushed.

Parametrical Study

❑ What are the main geometrical features which affect significantly the mechanical response of PU foams?

INPUT

1. Cell size distribution (Gaussian distribution, [μ,SD])
2. Strut shape (in form of 4^{th} order Polynomial function)
3. Foam density (Kg/m3)
4. Fraction of material in struts and walls
5. Anisotropy

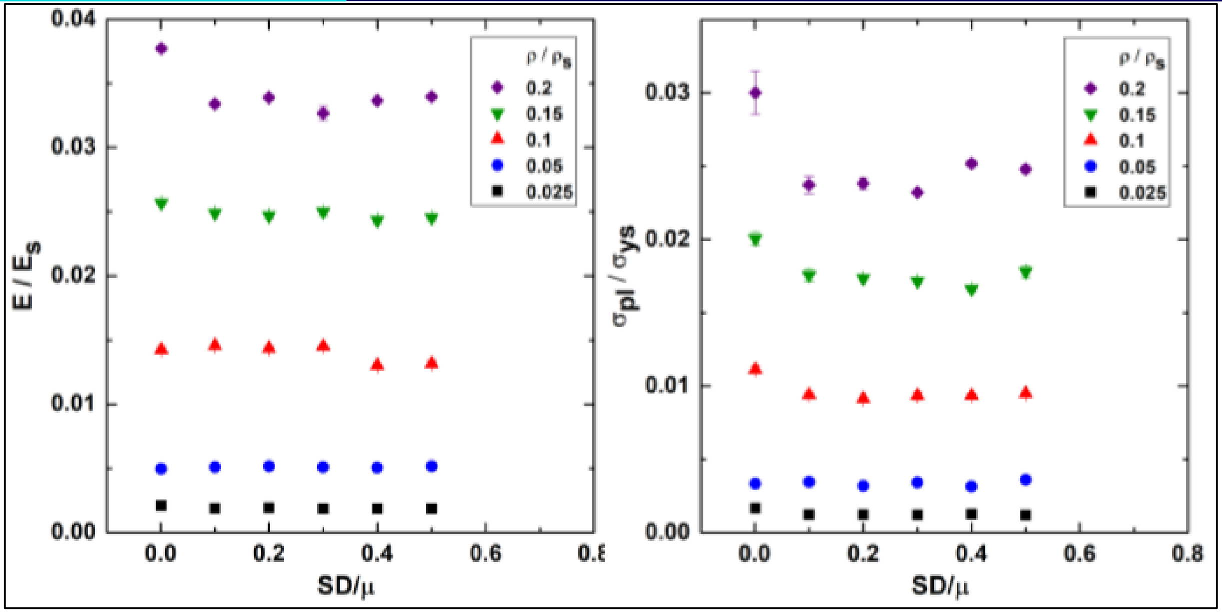
Output

- Foam stiffness
- Plateau stress

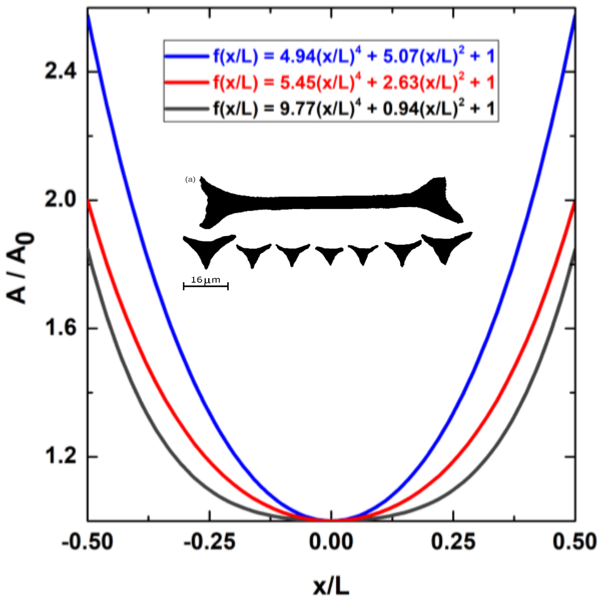
M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, "Surrogate models for the influence of the microstructure on the mechanical properties of close and open-cell foams", Journal of Materials Science, 53, pp 12937-12948, 2018.

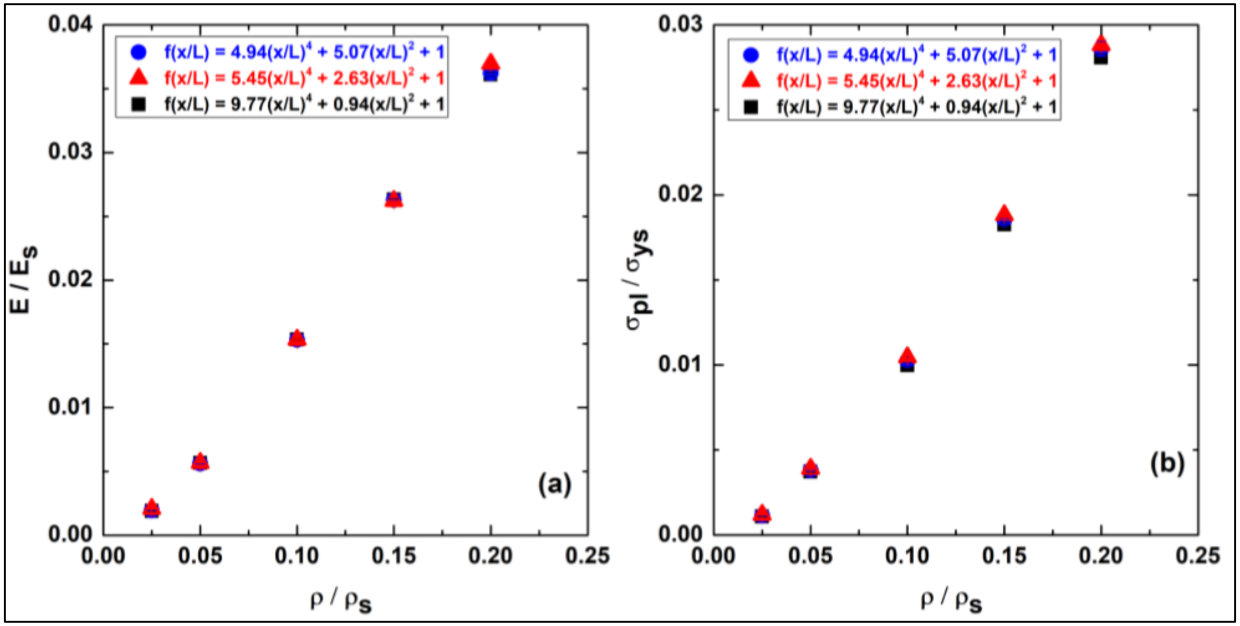
Parametrical Study

1. Cell size distribution



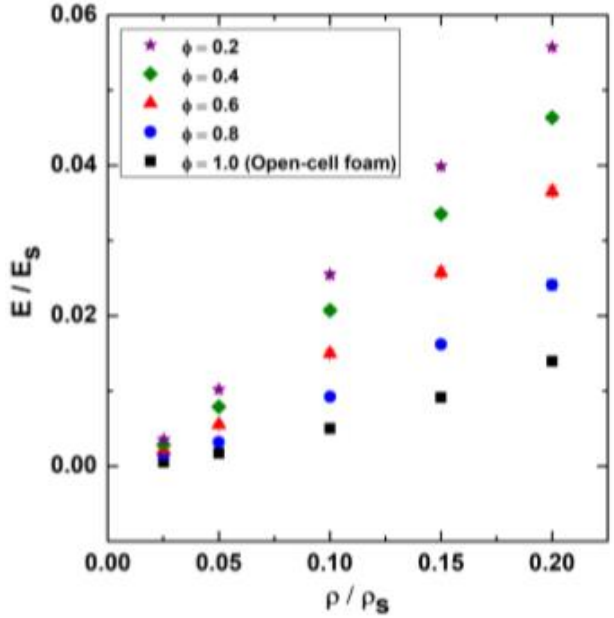
2. Strut shape

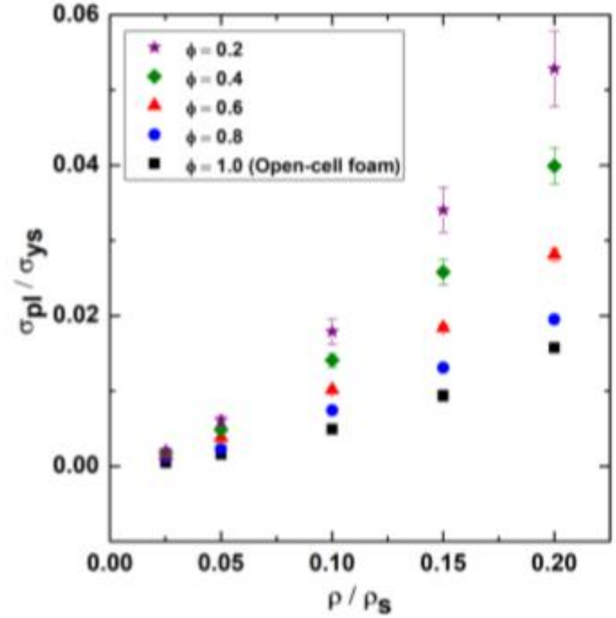




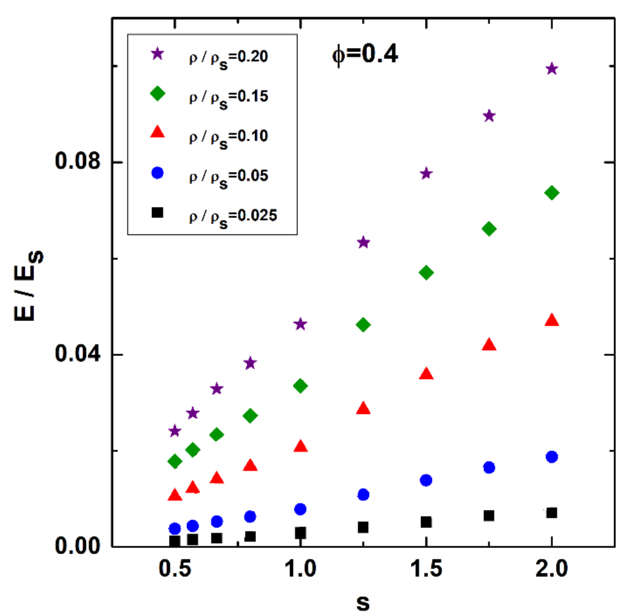
Parametrical Study

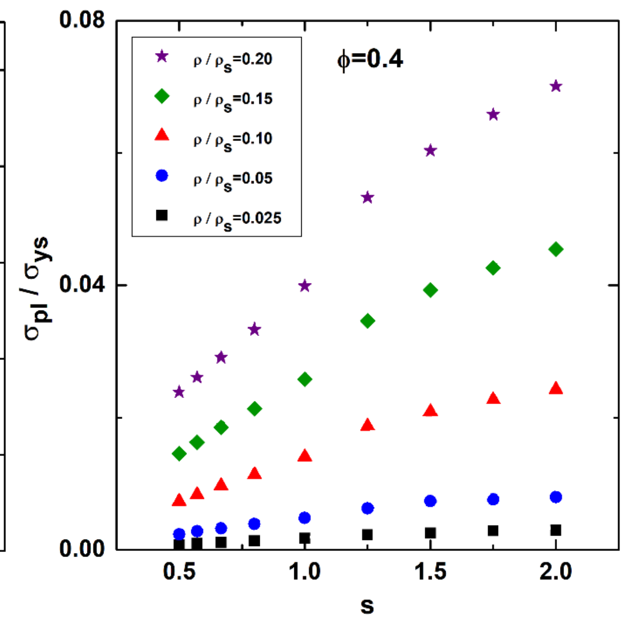
3. Foam density and strut contain





4. Anisotropy





Surrogate Models

Surrogate models to calculate the foam elastic modulus and plateau stress as a function of foam density, volume of material in walls and struts and cell aspect ratio.

Surrogate model for elastic modulus (E)

$$\frac{E}{E_s} = C_1 s^{1.2}\left(\phi \frac{\rho}{\rho_s}\right)^{1.5} + C_1' s^{1.1}(1-\phi)\left(\frac{\rho}{\rho_s}\right)^{1.2}$$

Surrogate model for Plateau stress

$$\frac{\sigma_{pl}}{\sigma_{ys}} = C_3 s^{0.6} \phi^{3.5}\left(\frac{\rho}{\rho_s}\right)^{1.5} + C_4 s^{0.8}(1-\phi)\left(\frac{\rho}{\rho_s}\right)^{1.5}$$

C_1	C_1'	C_3	C_4
0.158	0.5155	0.156	0.760

M. Marvi-Mashhadi, C. S. Lopes, J. LLorca, "Surrogate models for the influence of the microstructure on the mechanical properties of close and open-cell foams", Journal of Materials Science, 53, pp 12937-12948, 2018.

CONCLUSIONS

- A **modeling strategy** based on micromechanical characterization and computational homogenization of a representative volume of the microstructure has been developed to determine the mechanical behavior of **rigid, open and closed-cell PU foams**.
- The **viscoelastic properties** and **compressive flow stress** of the **solid PU** within the foam were determined by means of **nanoindentation**.
- Analyses showed that the **load** applied to the foam was **mainly supported by the struts**.
- The simulations explained the **large effect of anisotropy** in the mechanical response of the PU foams.
- The **parametric study** showed that the main geometrical features which affect significantly the mechanical response of PU foams are the **relative density**, the **distribution of solid PU between struts and walls** as well as the **cell anisotropy.**
- Based on calculated results, **new surrogate models** have been proposed for closed- and open-cell foams.

Future work

- Include the effect of internal pressure during deformation in the simulation to predict the mechanical response up to densification.
- Extension of modeling strategy to simulate the mechanical behavior of the foams in tension and shear and also at high temperature.

ACKNOWLEDGEMENT

MOdelling of morphology
DEvelopment of micro- and
NAnostructures (MoDeNa) FP7

SEVENTH FRAMEWORK PROGRAMME

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DIN

Thank you very much for your attention