Architectured materials

Design, fabrication and characterization

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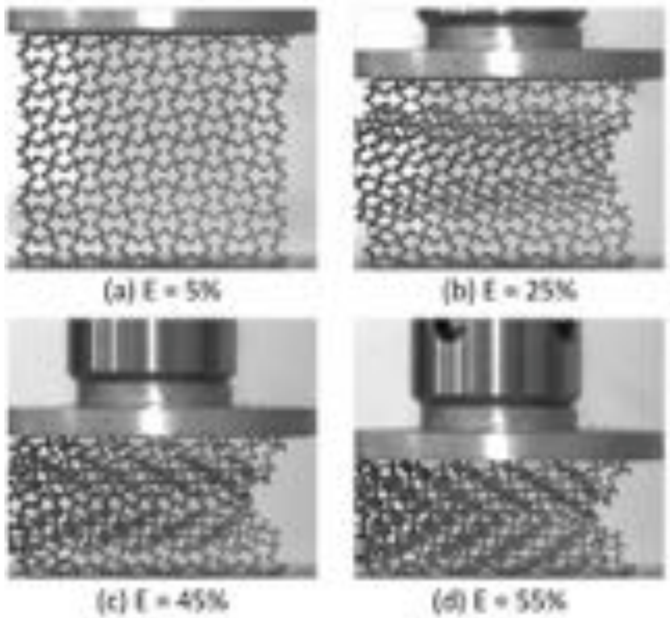
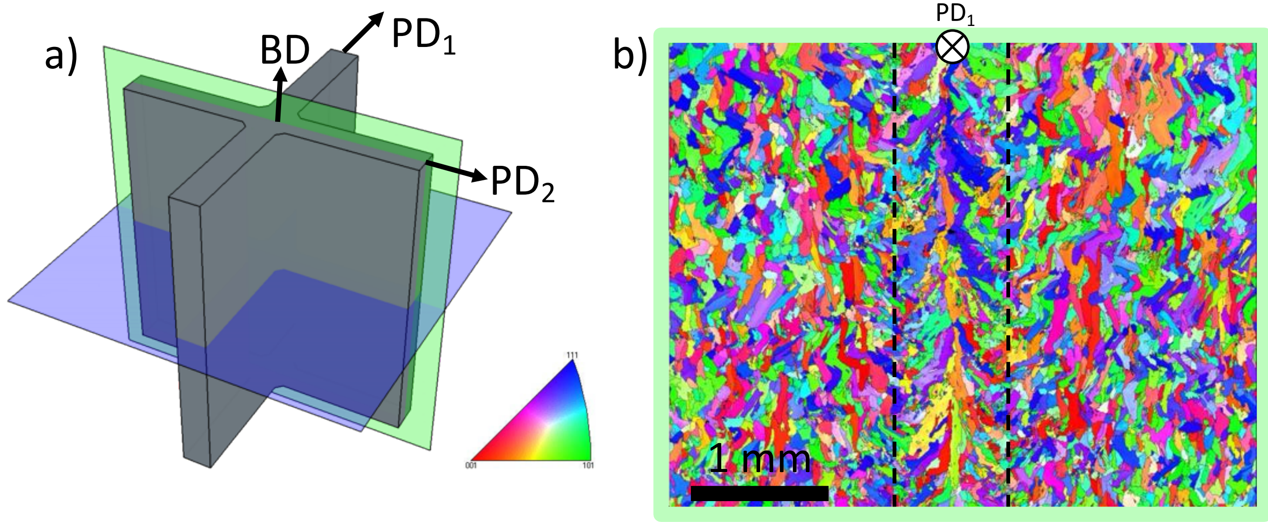
GDR ArchiMeta
2024 June 11

Architectured materials
Structures and Microstructures

Ordered



Random



Balit et al. https://doi.org/10.1016/j.mechmat.2021.103915

Outline

Ordered [micro]structures

Topological shape optimisation

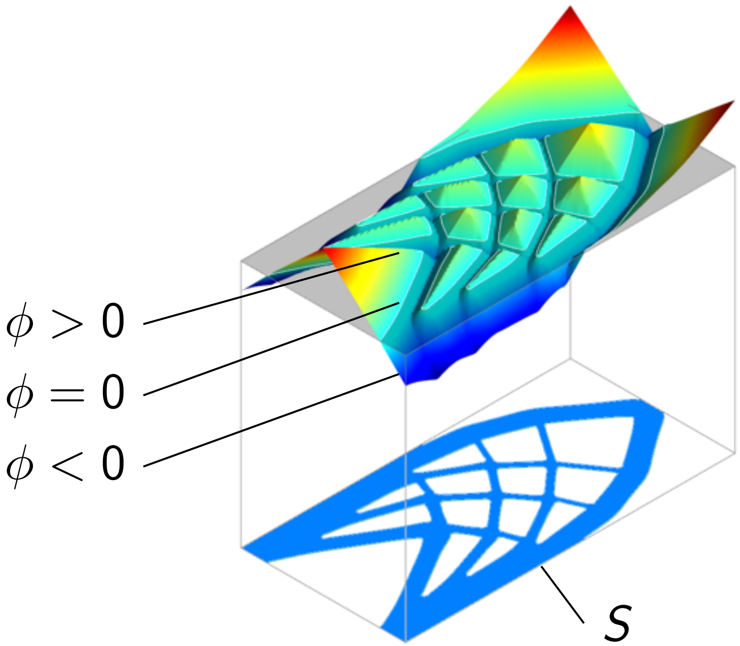
- Shape derivative with level set function
- Examples
  - 2D multilayer materials
  - Panels with periodic microstructure
  - Thick shells with IGA

Random microstructures

- Morphology and regularity : topology and randomness
- Example
  - Lattice with surface roughness
  - Random cellular materials

Implicitly-defined Shape

Level Set Method

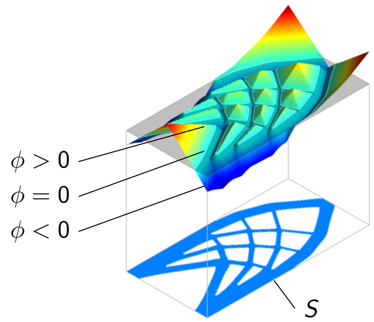


$$\begin{cases} \phi(\mathbf{x}) < 0 & \text{if} \quad \mathbf{x} \in S & \text{(material)} \\ \phi(\mathbf{x}) = 0 & \text{if} \quad \mathbf{x} \in \partial S & \text{(boundary)} \\ \phi(\mathbf{x}) > 0 & \text{if} \quad \mathbf{x} \in \mathcal{D} \setminus S & \text{(void)} \end{cases}$$

$$\mathbf{n}(\mathbf{x}) = \frac{\nabla \phi(x)}{|\nabla \phi(x)|}.$$

Implicitly-defined Shape

Shape evolution



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$S(t)$

$$\phi(t, \mathbf{x}(t)) = 0, \qquad \forall t \in [0, T].$$

$$\frac{\partial \phi}{\partial t}(t, \mathbf{x}) + \dot{\mathbf{x}}(t) \cdot \nabla \phi(t, \mathbf{x}) = 0, \qquad \forall t, \ \forall \mathbf{x} \in \partial S(t).$$

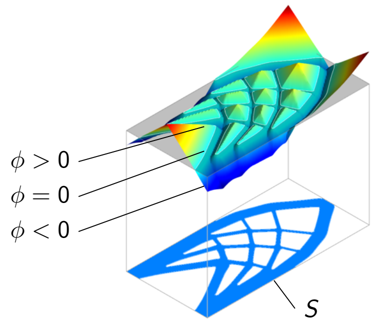
$$\frac{\partial \phi}{\partial t}(t, \mathbf{x}) + \boldsymbol{\theta}(t, \mathbf{x}(t)) \cdot \nabla \phi(t, \mathbf{x}) = 0, \qquad \forall t, \ \forall \mathbf{x} \in \partial S(t), \qquad \boldsymbol{\theta}(t, \mathbf{x}) = V(t, \mathbf{x})\, \mathbf{n}(t, \mathbf{x}),$$

Hamilton-Jacobi

$$\boxed{\frac{\partial \phi}{\partial t}(t, \mathbf{x}) + V(t, \mathbf{x}) \left| \nabla \phi(t, \mathbf{x}) \right| = 0, \qquad \forall t, \ \forall \mathbf{x} \in \mathcal{D}.}$$

Shape optimization

Algorithm



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Data: Initialise a level set function ϕ_0 corresponding to an initial shape S^0;

for $k \geq 0$ *iterate until convergence* **do**

- Redistance ϕ_k into the signed distance function d_{S^k} using eq. (2.4.9);
- Compute $\mathbf{u}_k$ and $\mathbf{p}_k$, solutions of the state (2.3.9) and adjoint (2.3.10) equations for the domain S^k;
- Compute the shape gradient $\mathcal{J}(S^k)(\theta^k)$ for the domain S^k using eq. (2.4.13);
- Deform the domain S^k by solving the Hamilton-Jacobi equation (2.4.6);
  // Shape S^{k+1} is characterised by the level set ϕ_{k+1} after a time step Δt_k
  // The time step Δt_k is chosen so that $\mathcal{J}(S^{k+1}) \leq \mathcal{J}(S^k)$

end

Multilayer Materials

Optimised microstructures - Poisson ratio

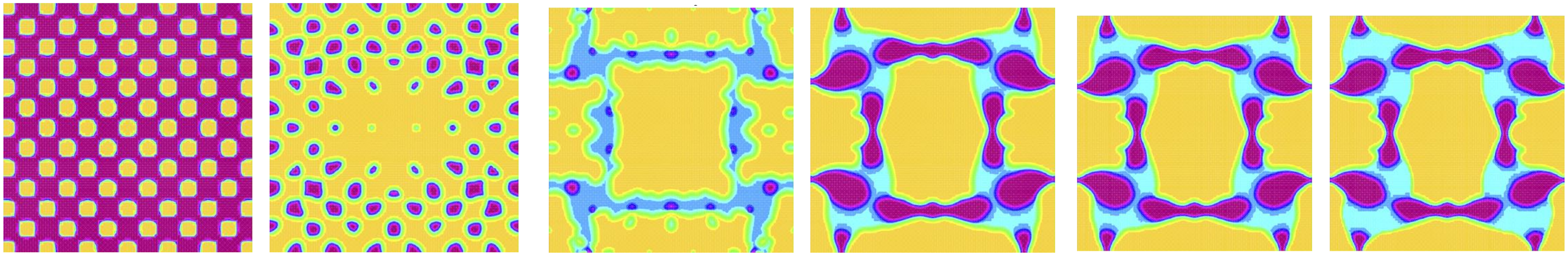
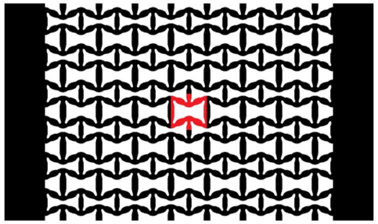


Fig. 7. Example 1: The design process of the multi-layer material at different iteration steps in the design domain Y. The unit cell was optimized so that the resulting macro-structure attains an apparent Poisson's ratio $\nu^* = -1$. The different colors represent the different Young moduli of the material: ● Young modulus of 1.82, ● Young modulus of 0.91, ● void.

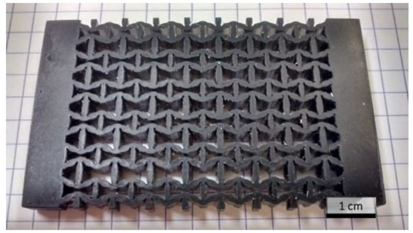
Optimal Poisson ratio

Plane orthotropic materials

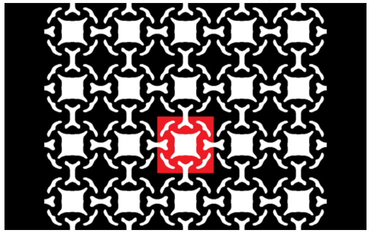
$\mathbb{C}^t$	$\mathbb{C}^H(\omega)$	ν^t	ν^H	Shape ω
$\begin{bmatrix} 0.1 & -0.1 & 0 \\ -0.1 & 0.1 & 0 \\ 0 & 0 & G \end{bmatrix}$	$\begin{bmatrix} 0.12 & -0.05 & 0 \\ -0.05 & 0.04 & 0 \\ 0 & 0 & 0.006 \end{bmatrix}$	$-1.$	$\{-1.25, -0.42\}$	
$\begin{bmatrix} 0.1 & -0.1 & 0 \\ -0.1 & 0.1 & 0 \\ 0 & 0 & G \end{bmatrix}$	$\begin{bmatrix} 0.12 & -0.05 & 0 \\ -0.05 & 0.12 & 0 \\ 0 & 0 & 0.003 \end{bmatrix}$	$-1.$	-0.42	
$\begin{bmatrix} 0.2 & -0.1 & 0 \\ -0.1 & 0.2 & 0 \\ 0 & 0 & G \end{bmatrix}$	$\begin{bmatrix} 0.19 & -0.09 & 0 \\ -0.09 & 0.19 & 0 \\ 0 & 0 & 0.6 \end{bmatrix}$	-0.5	-0.47	



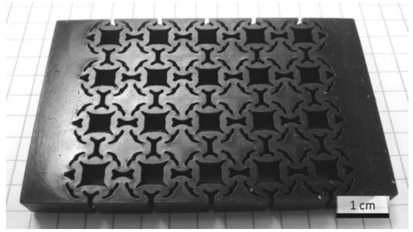
Example 1: Input design



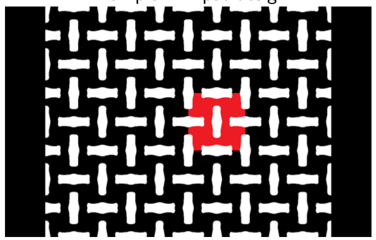
Example 1: Fabricated result



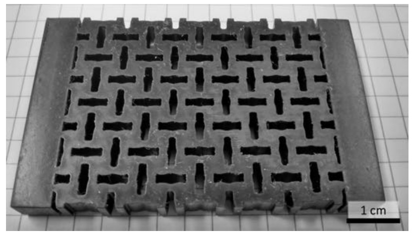
Example 2: Input design



Example 2: Fabricated result



Example 3: Input design



Example 3: Fabricated result

Multilayer Materials

2D plane orthotropic

$$\begin{pmatrix} \Sigma_{11} \\ \Sigma_{22} \\ \Sigma_{12} \end{pmatrix} = \begin{pmatrix} C^*_{1111} & C^*_{1122} & 0 \\ C^*_{1122} & C^*_{2222} & 0 \\ 0 & 0 & C^*_{1212} \end{pmatrix} \begin{pmatrix} \varepsilon_{\mathbf{x}11} \\ \varepsilon_{\mathbf{x}22} \\ 2\,\varepsilon_{\mathbf{x}12} \end{pmatrix}$$

$$\begin{pmatrix} \varepsilon_{\mathbf{x}11} \\ \varepsilon_{\mathbf{x}22} \\ 2\,\varepsilon_{\mathbf{x}12} \end{pmatrix} = \begin{pmatrix} 1/E^*_1 & -\nu^*_{12}/E^*_1 & 0 \\ -\nu^*_{21}/E^*_2 & 1/E^*_2 & 0 \\ 0 & 0 & 1/G^*_{12} \end{pmatrix} \begin{pmatrix} \Sigma_{11} \\ \Sigma_{22} \\ \Sigma_{12} \end{pmatrix}$$

$$\frac{\nu^*_{12}}{E^*_1} = \frac{\nu^*_{21}}{E^*_2}.$$

$$C^*_{1111} = \frac{E^*_1}{1-\nu^*_{12}\nu^*_{21}}, \qquad C^*_{2222} = \frac{E^*_2}{1-\nu^*_{12}\nu^*_{21}}, \qquad C^*_{1122} = \frac{\nu^*_{21}\,E^*_1}{1-\nu^*_{12}\nu^*_{21}}.$$

$$\nu^*_{12} = \frac{C^*_{1122}}{C^*_{2222}}, \qquad \nu^*_{21} = \frac{C^*_{1122}}{C^*_{1111}}.$$

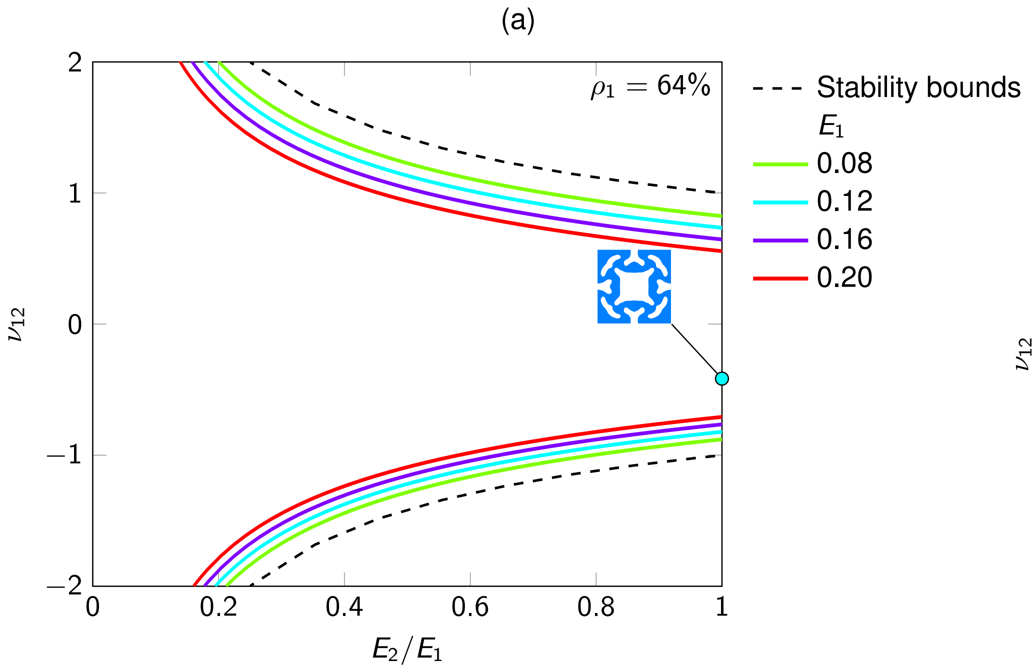
Stability Bounds

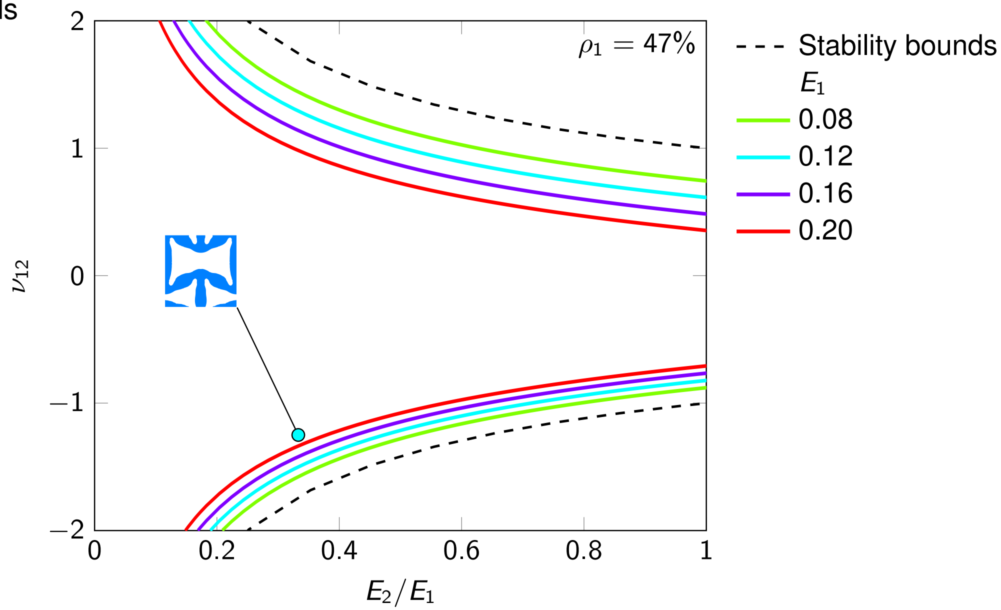
$$|\nu_{12}| \le \sqrt{\frac{E_1}{E_2}}, \qquad |\nu_{21}| \le \sqrt{\frac{E_2}{E_1}}, \qquad 1-\nu_{12}\,\nu_{21} > 0.$$

Optimal Poisson ratio

Plane orthotropic materials

Milton Kohn Bounds

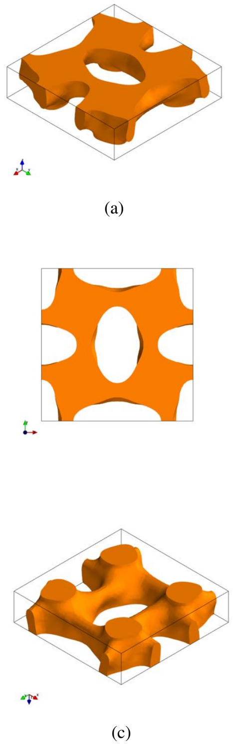


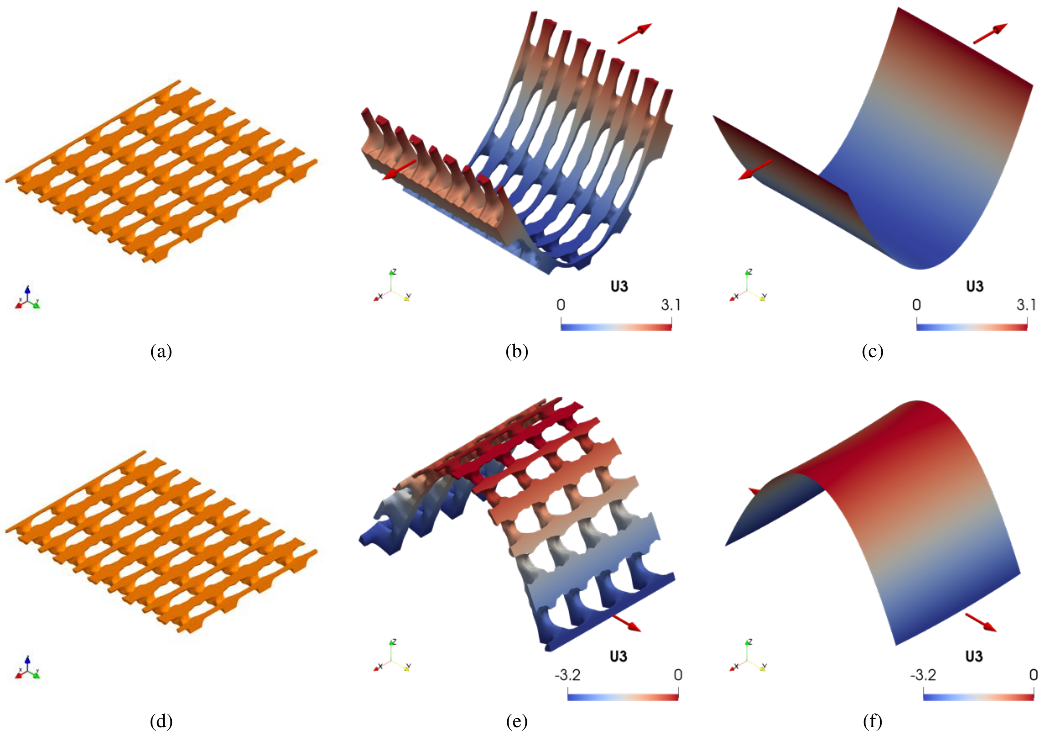


Agnelli - PhD Thesis 2021

Panels

Optimised microstructure for Extention - Bending Coupling





Agnelli et al. CMAME 2022

Panels

Optimised microstructure for Extention - Bending Coupling

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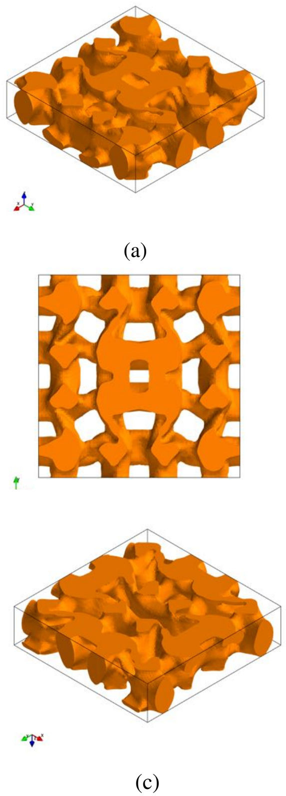

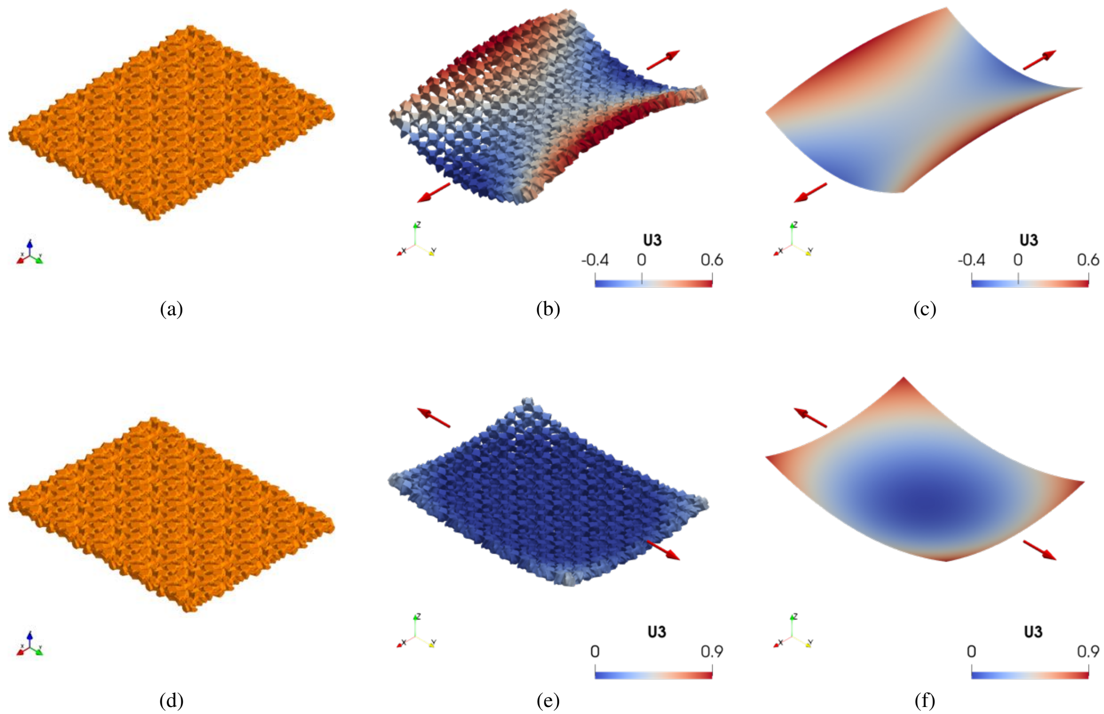

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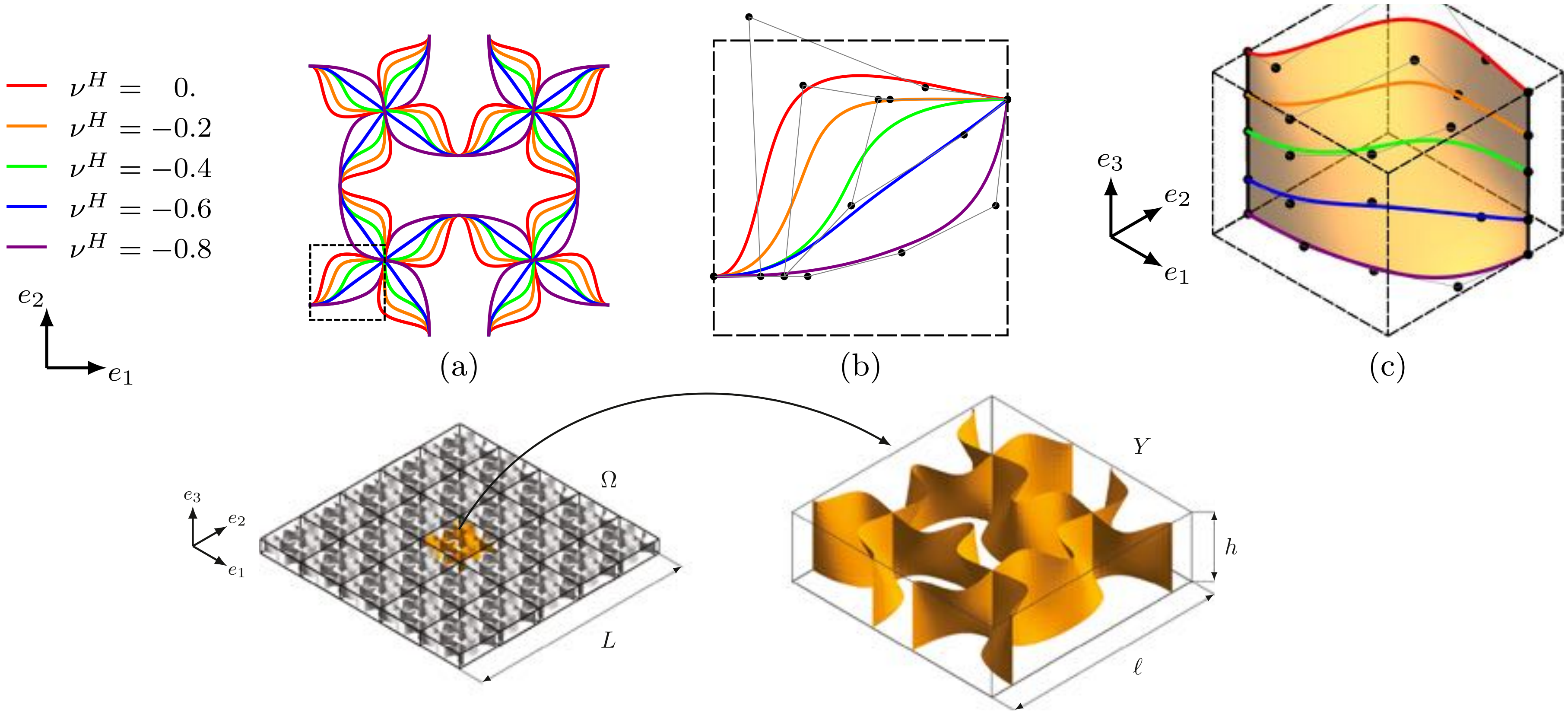
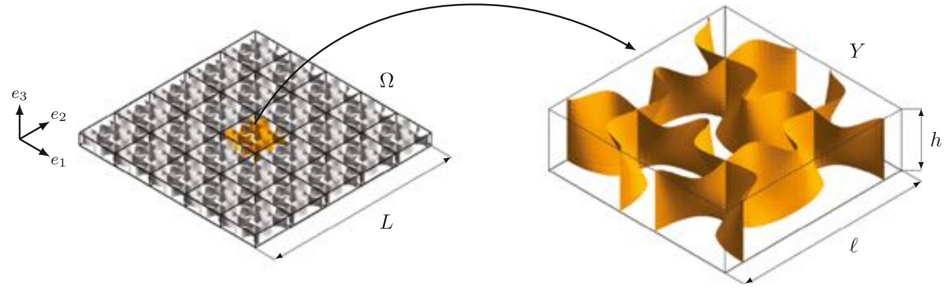
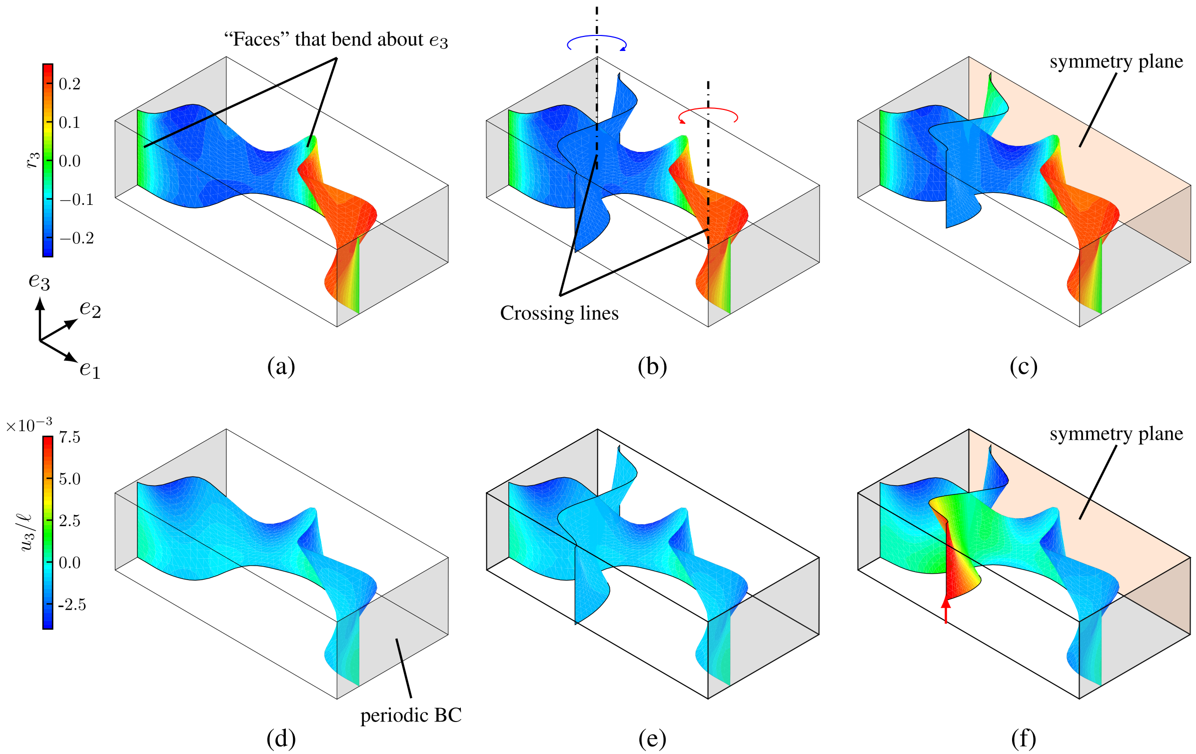
Ribbon Network



Agnelli et al. doi.org/10.1016/j.eml.2020.101089

Ribbon Network

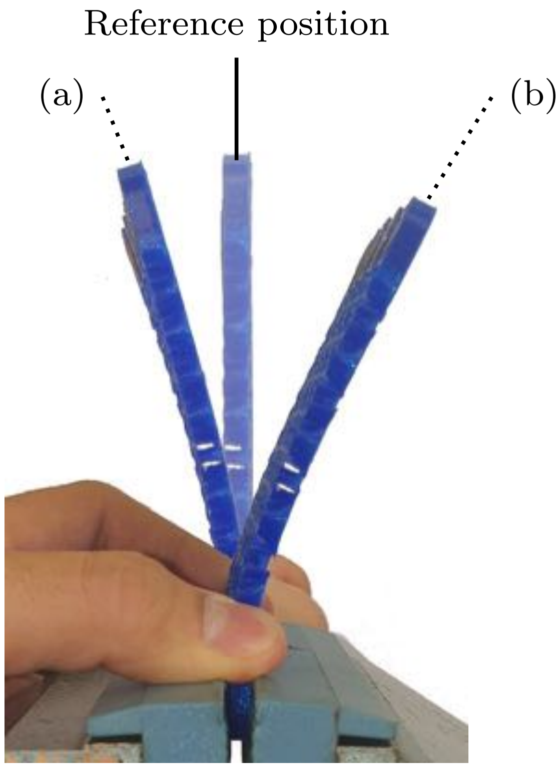


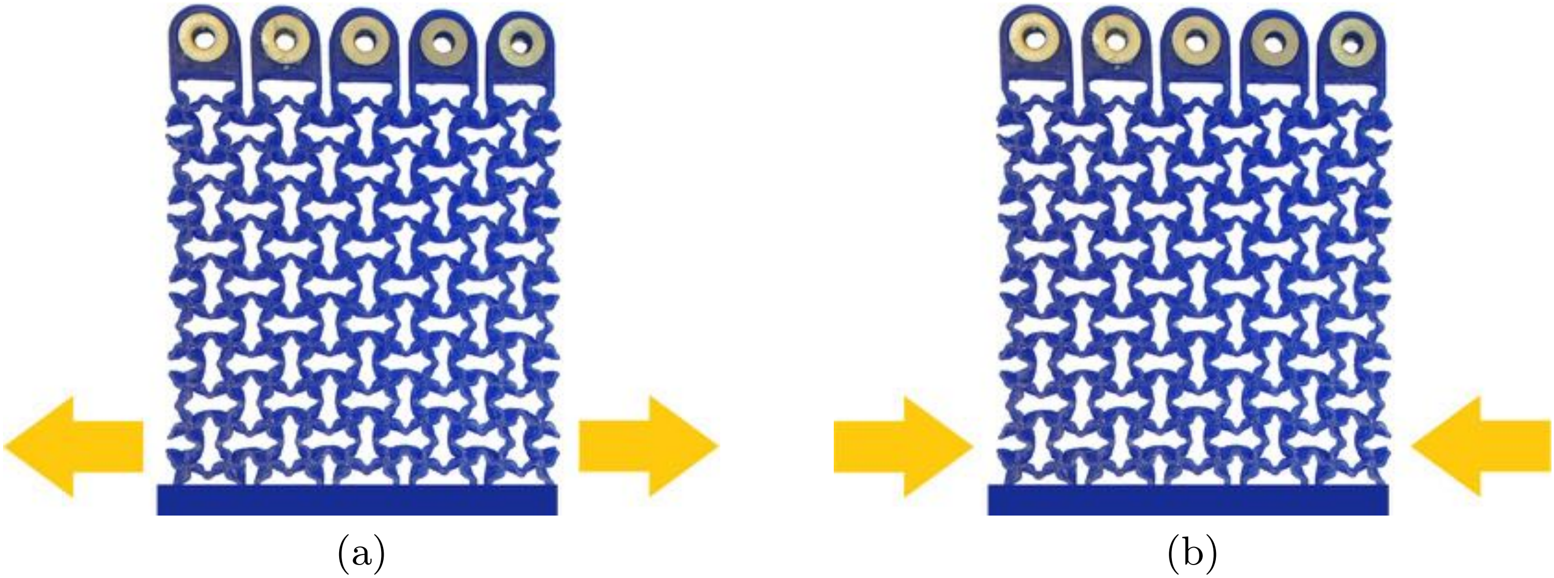


Agnelli et al. doi.org/10.1016/j.eml.2020.101089

Shape shifting

ribbon structures

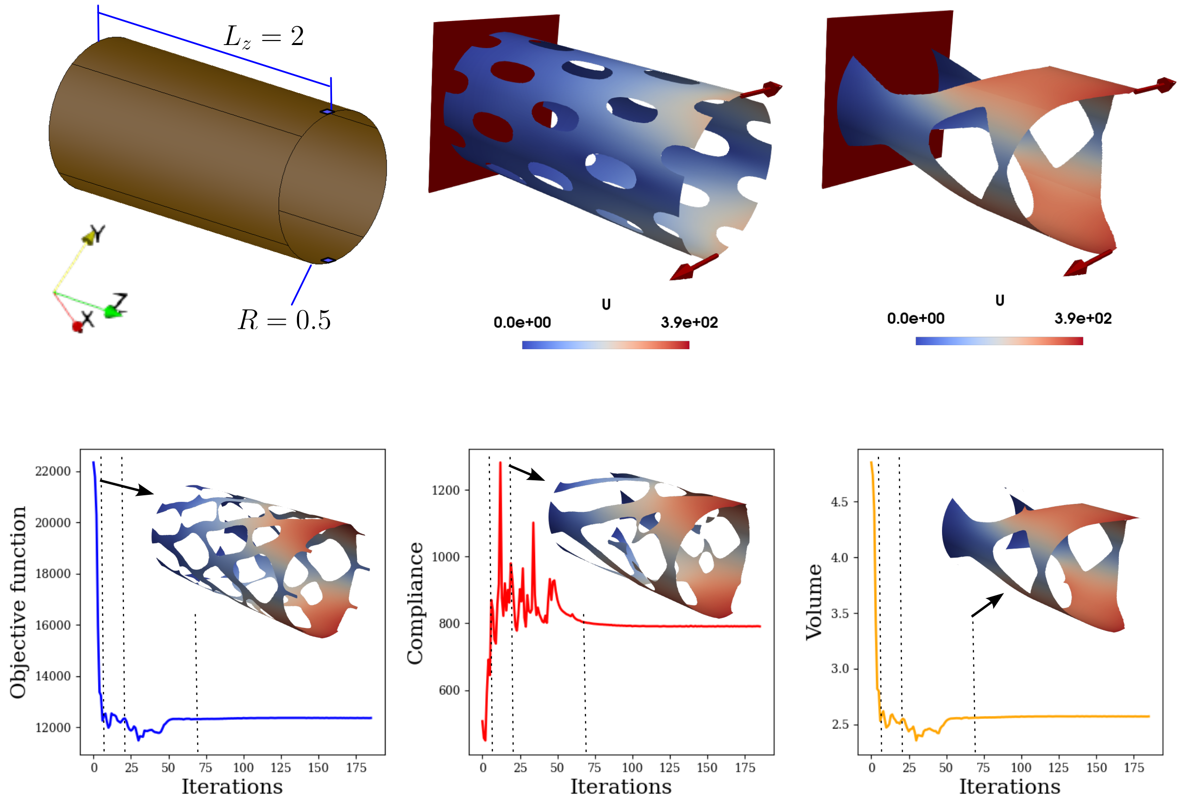




Agnelli, Tricarico, Constantinescu.*arXiv preprint arXiv:2009.09741* (2020).

Isogeometric Analysis - Thick Shell

Stiffness Optimization with volume constraint



Hubner-Scherer et al. Submitted CMAME 2024

Outline

Ordered [micro]structures

Topological shape optimisation

- Shape derivative with level set function
- Examples
  - 2D multilayer materials
  - Panels with periodic microstructure
  - Thick shells with IGA

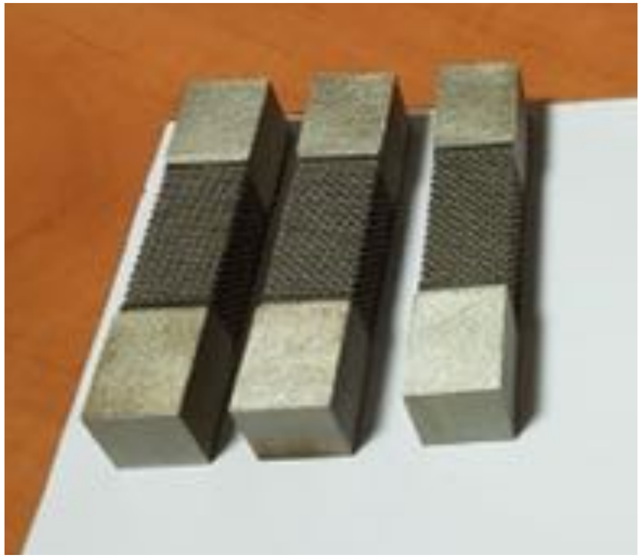
Random microstructures

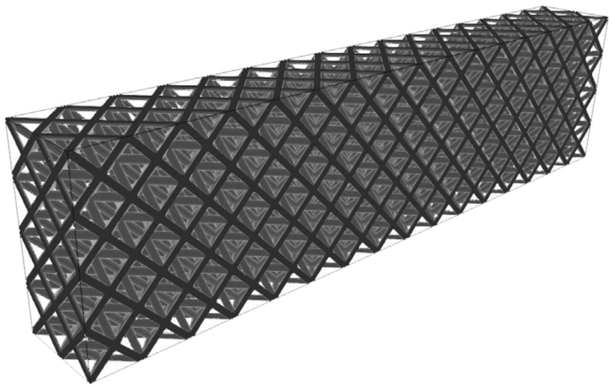
- Morphology and regularity : topology and randomness
- Example
  - Lattice with surface roughness
  - Random cellular materials

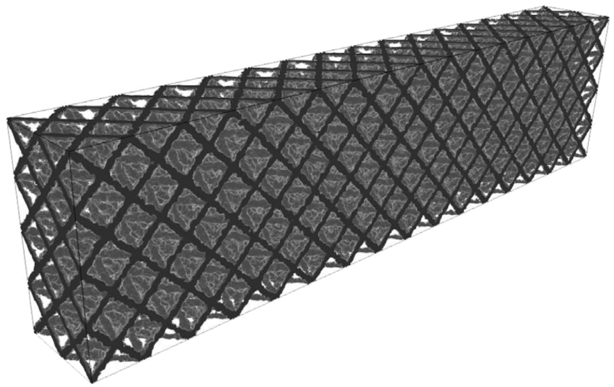
Architectured lattice

Level set

Topological support and randomness



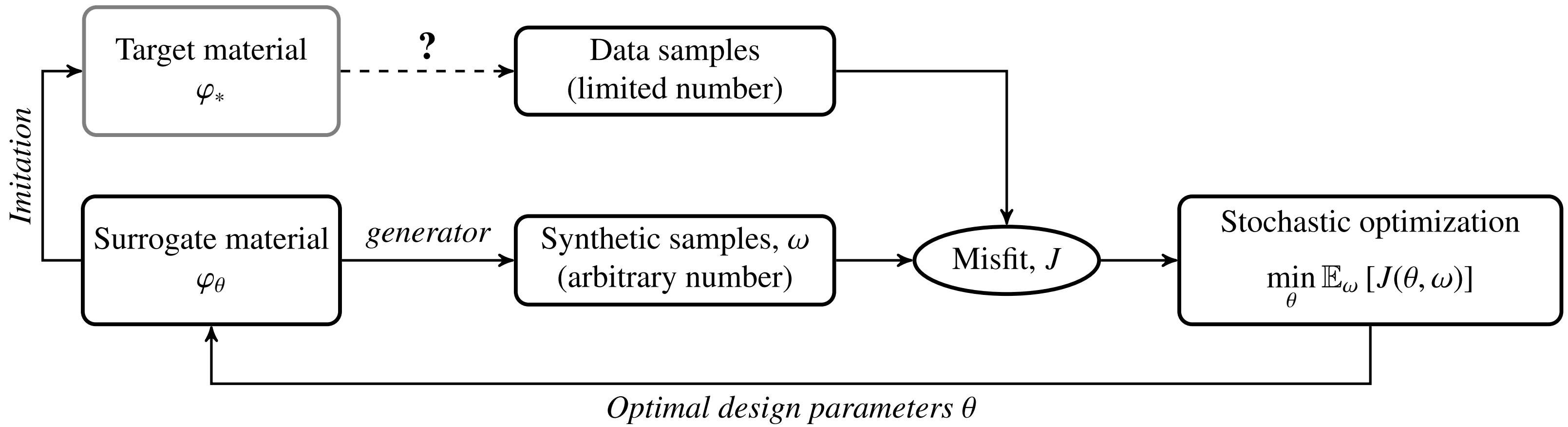




$$\phi(x;\theta,\omega) = (1-\alpha)\cdot\phi_1(x;\theta,\omega) + \alpha\cdot\phi_2(x;\theta,\omega)$$

Khistenko et al. CMAME 2022

Material parameters
Level set : Topological support and randomness



- Stochastic Optimization
  - Bayesian Inference
    - PYMC, https://www.pymc.io/
  - Cost functional
    - Misfit of Two Point Correlation, Lineal Path, ...

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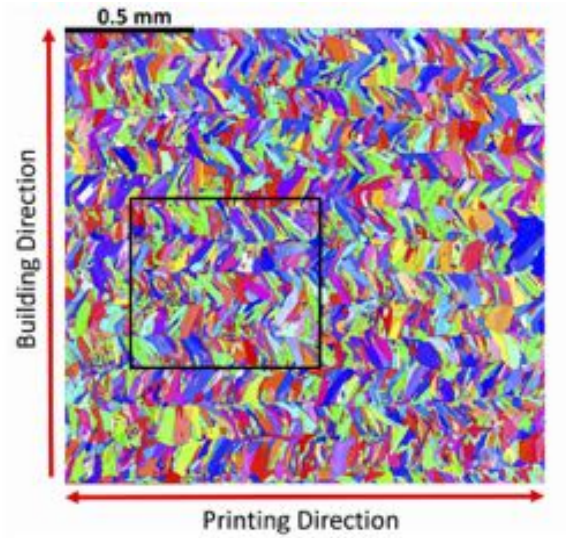
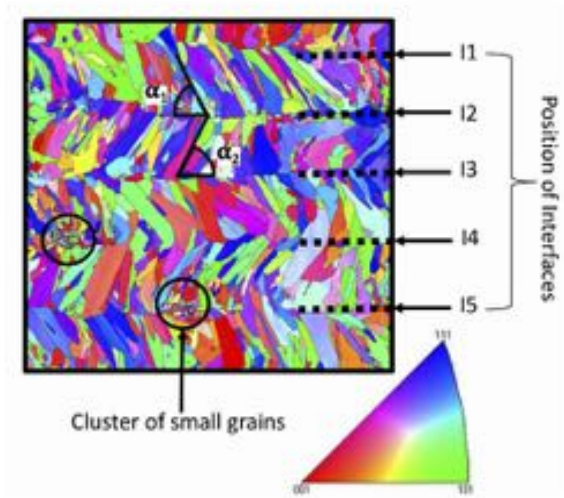
Material Morphology





geometrical descriptors

$$J(\theta, \omega) = \frac{1}{2} \sum_i \frac{\|d_i(\varphi_\theta(\omega)) - d_i^*\|^2}{\|d_i^*\|^2},$$

$$\min_\theta \mathbb{E}_\omega \left[J(\theta, \omega) \right],$$

$$d_1(\varphi) = \int_\Omega \varphi(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x},$$
$$d_2(\varphi) = \int_\Omega |\nabla \varphi(\boldsymbol{x})|\, \mathrm{d}\boldsymbol{x},$$
$$d_3(\varphi; \boldsymbol{r}) = \int_\Omega [\varphi(\boldsymbol{x} + \boldsymbol{r}) - d_1(\varphi)] \cdot [\varphi(\boldsymbol{x}) - d_1(\varphi)]\, \mathrm{d}\boldsymbol{x},$$
$$d_4(\varphi; \boldsymbol{r}) = \int_\Omega [|\nabla \varphi(\boldsymbol{x} + \boldsymbol{r})| - d_2(\varphi)] \cdot [|\nabla \varphi(\boldsymbol{x})| - d_2(\varphi)]\, \mathrm{d}\boldsymbol{x},$$

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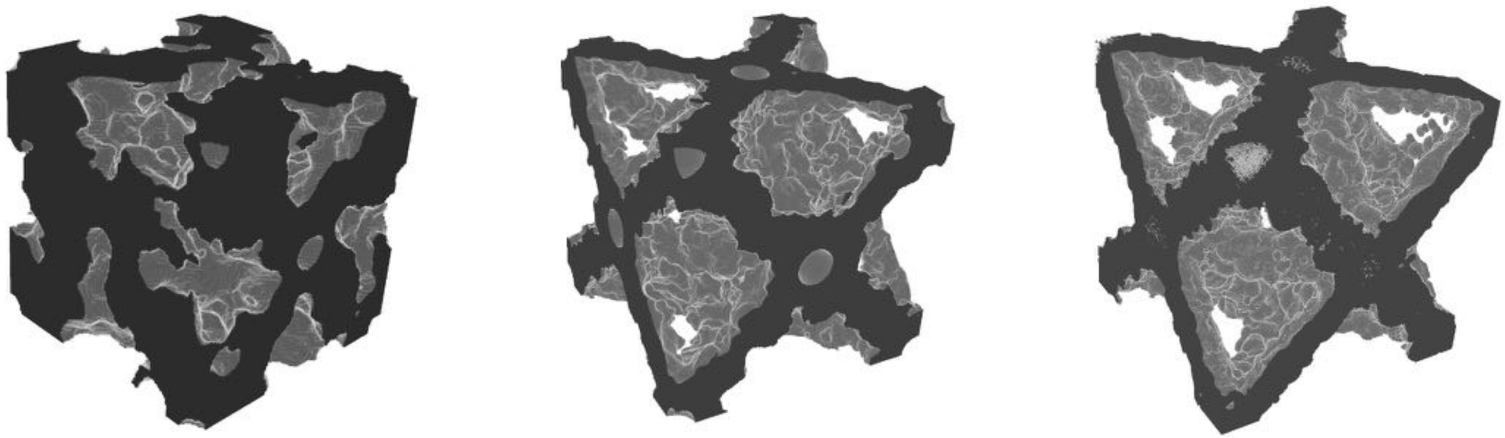
Architectured lattice

Level set

Topological support and randomness



(a) (b) (c)

Artificial Microstructures | **X-Ray Tomography**

$1\,nm$ $1\,\mu m$ $1\,cm$ Length Scale

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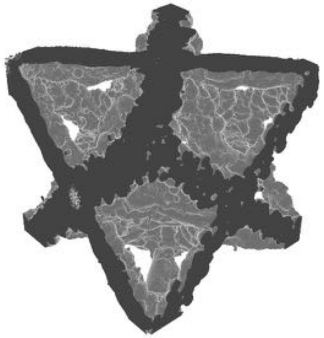
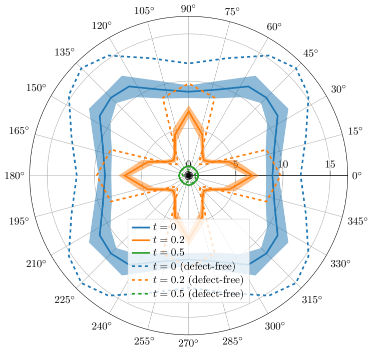
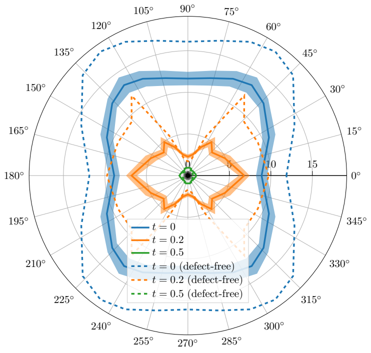
Architectured lattice

Elasto-plastic material behaviour

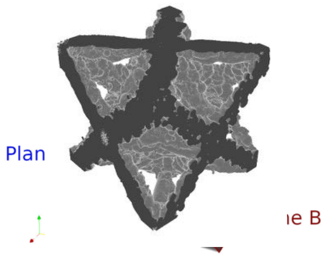




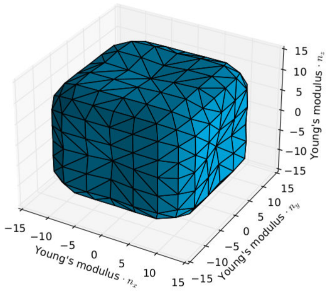
(a) Plane A



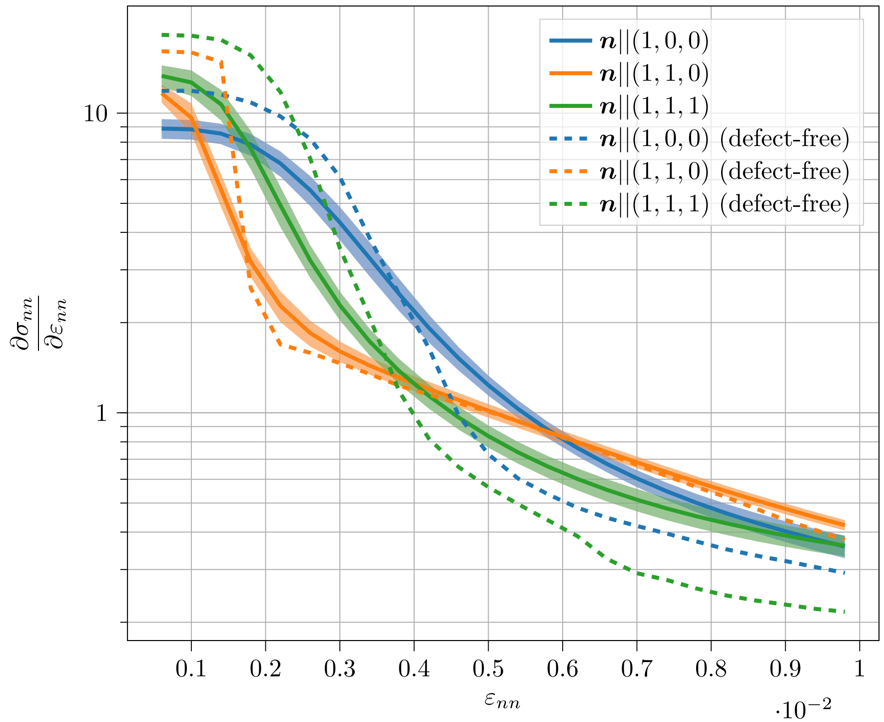
(b) Plane B



(c) Scheme of the cross-sections



(d) Young's modulus of the defect-free structure



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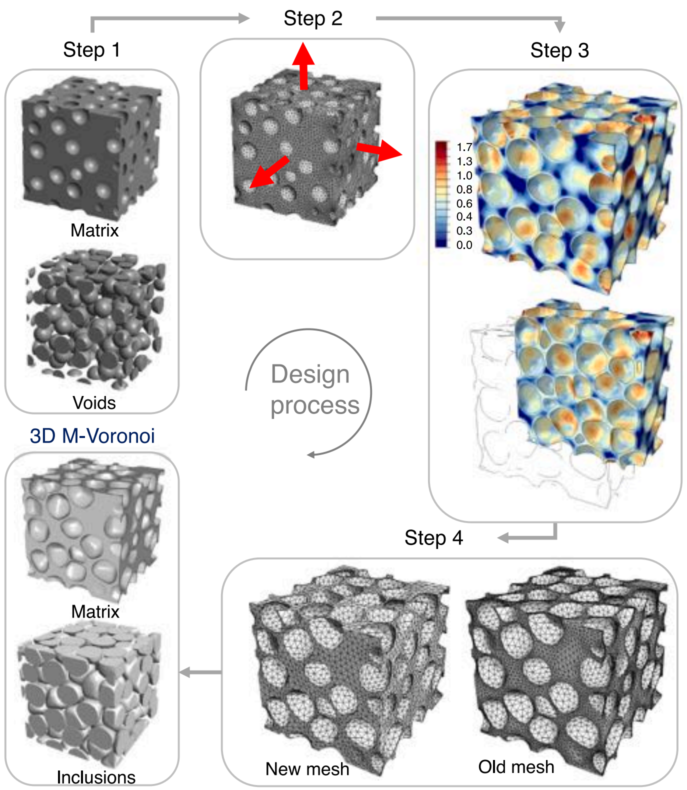
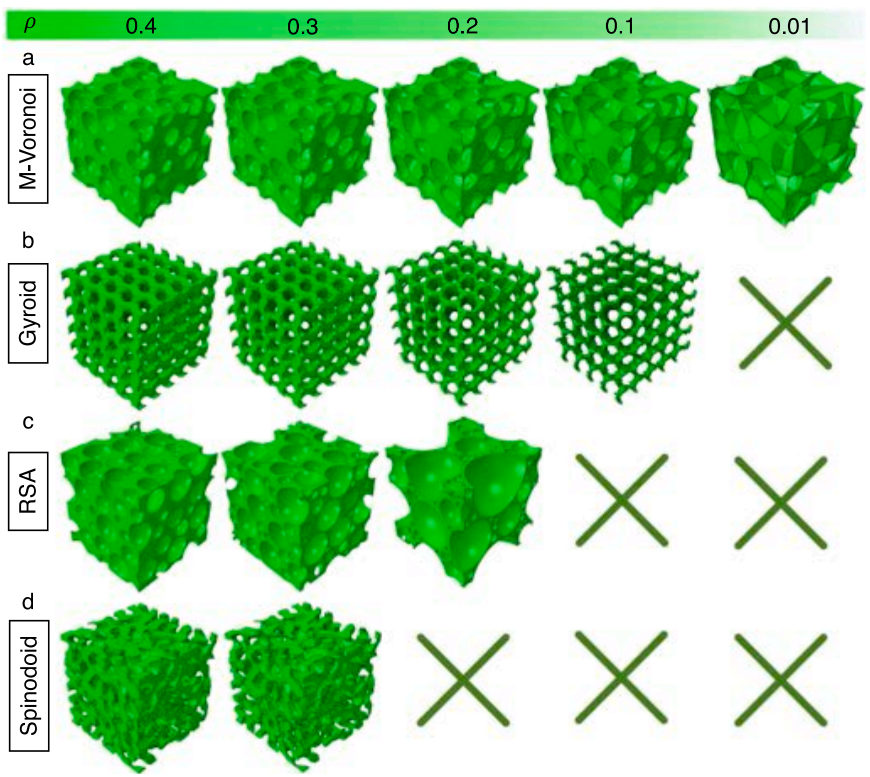
Cellular Materials

ordred or random: geometry generation

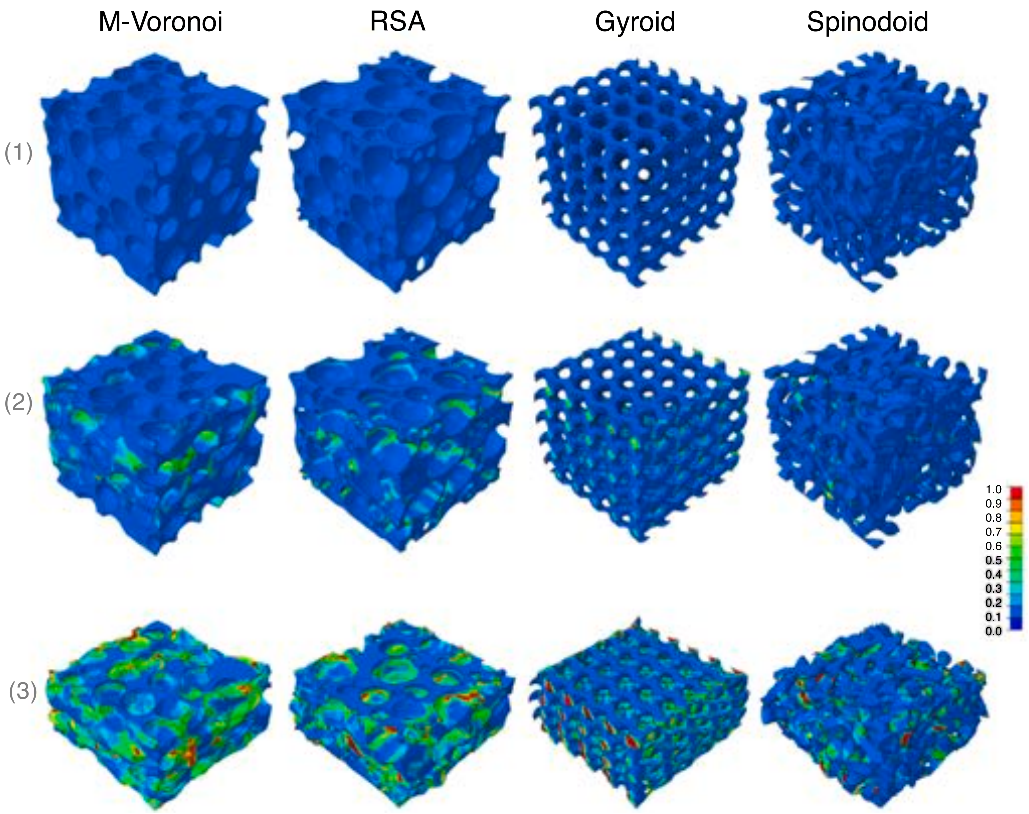


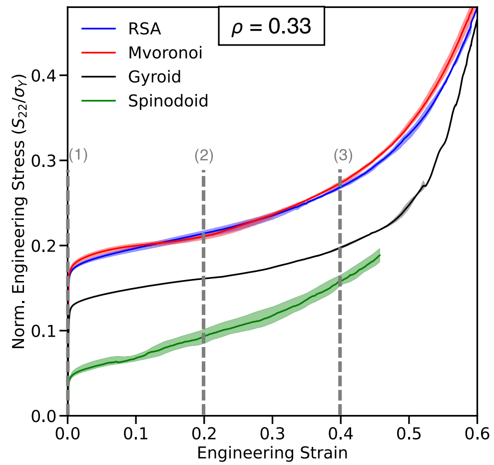


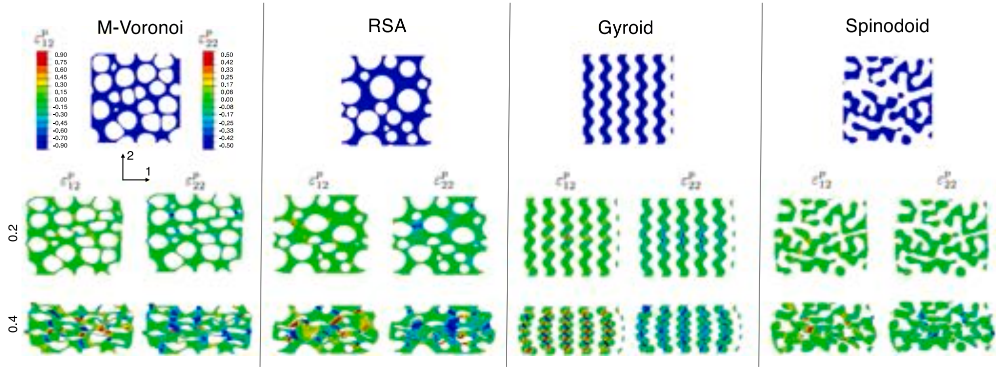
Hooshmand-Ahoor et al. IJSS 2024

Cellular Materials

Large strain compression







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Cellular Materials

Property map

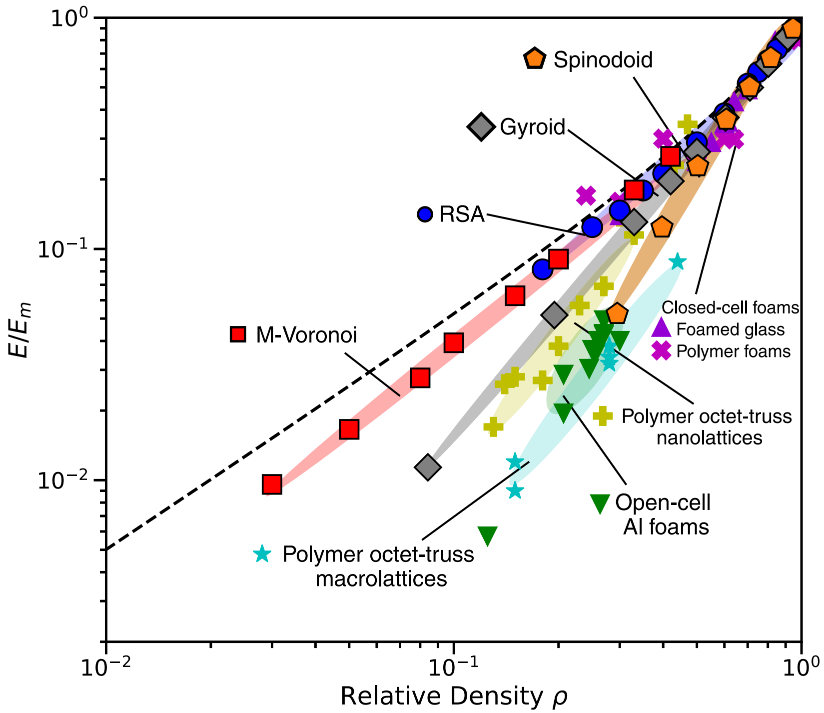
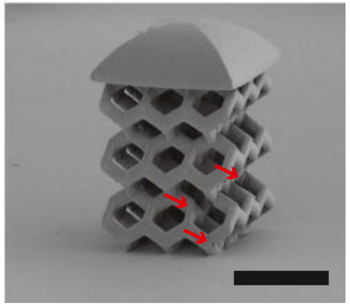
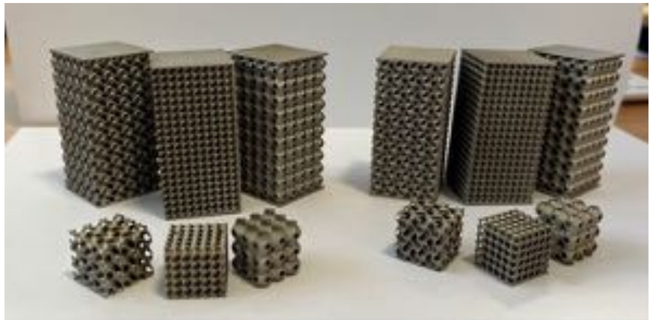
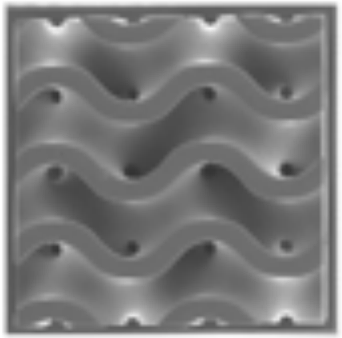
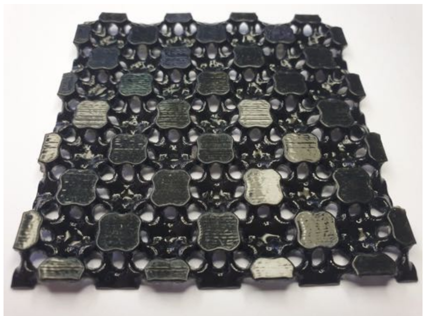


Fig. 6. A property space map of Young's modulus versus relative density ρ comparing the present geometries of M-Voronoi, RSA, Gyroid, and Spinodoid to other closed- and open-cell foams of similar density and to nano- and macro-lattices.

Hooshmand-Ahoor et al. IJSS 2024

Materials and microstructures

μm mm

- Polymer
- Metals
- Composites - MRE

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Eric Charkaluk
Kostas Danas
Julie Diani
Patrick Le Tallec

Andrei Constantinescu

Conclusions & Perspectives

- Optimal architectures
- Effect of randomness

- What properties can be reached ?
- What is printable ?