Microstructure Synthesis via Neural Networks

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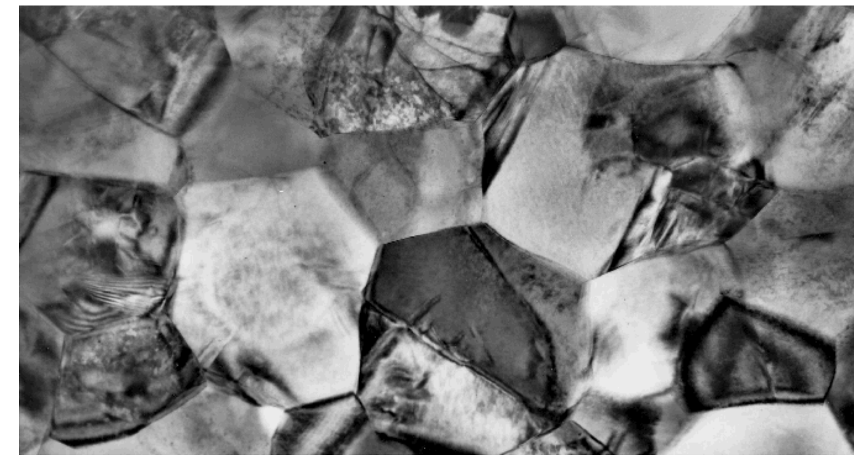
Background

Microstructure - structure, that can be observed under the microscope

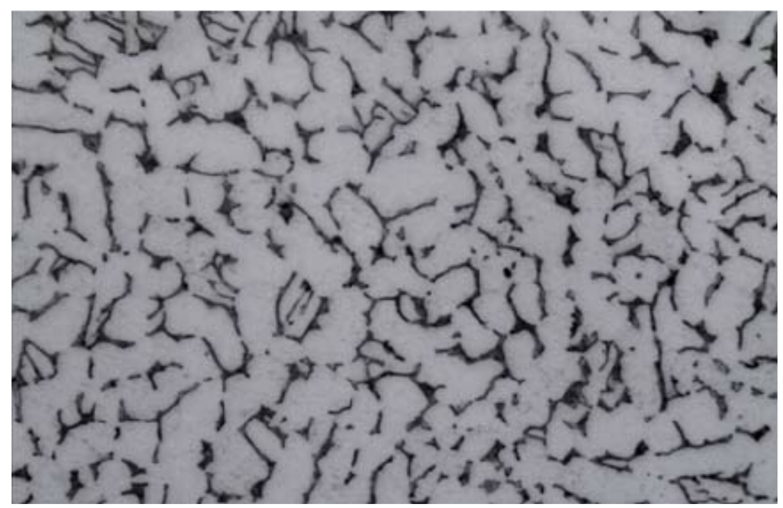
Microstructures are studied in:

- Medicine
- Space technologies
- Oil industry

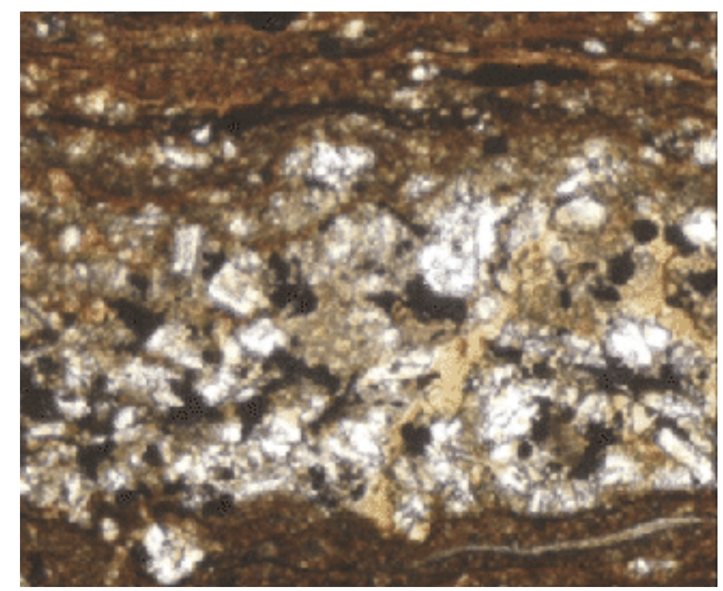
The problem – upscaling



Ceramics



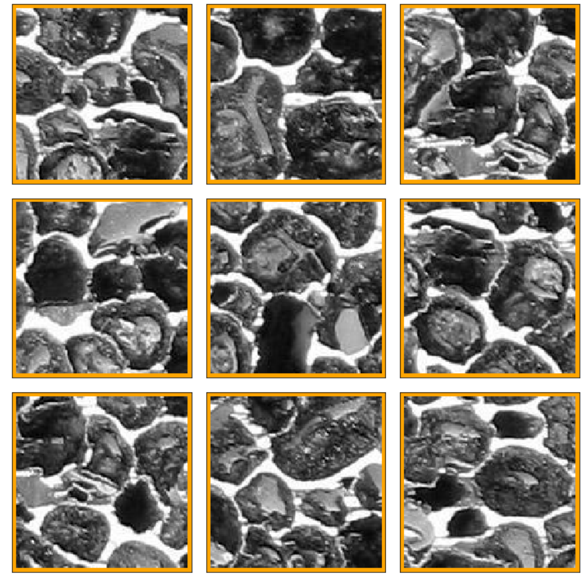
Titanium alloy



Soil slice

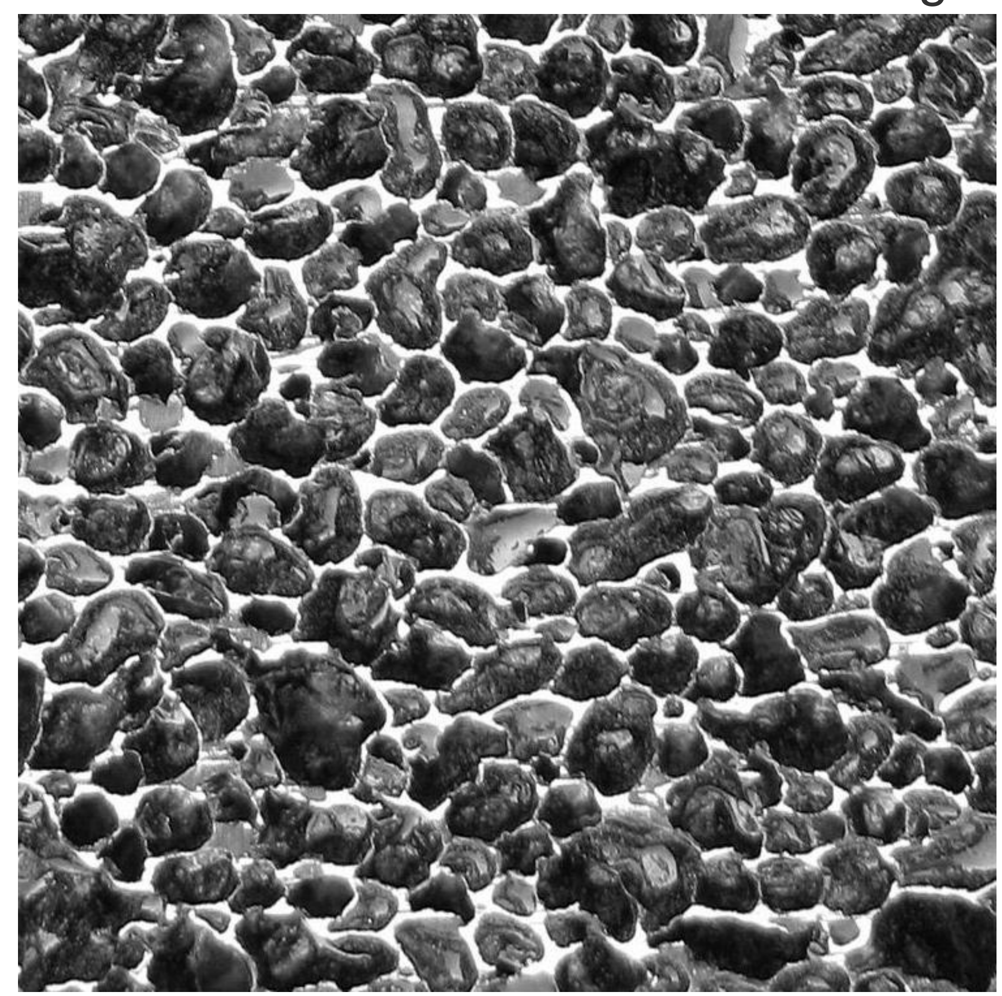
https://www.doitpoms.ac.uk
https://www.researchgate.net
https://www.researchgate.net

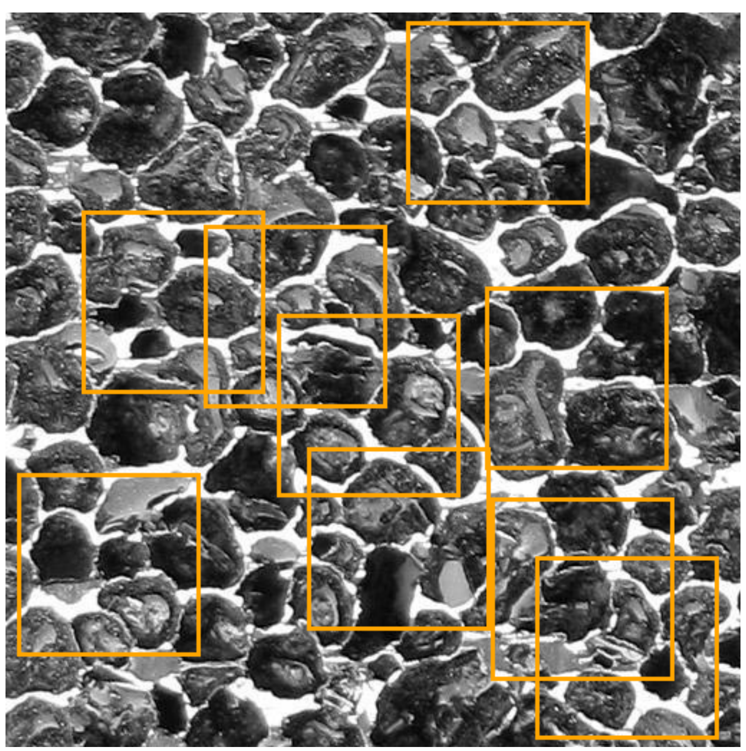
Aim



Random cuts

Reconstructed image





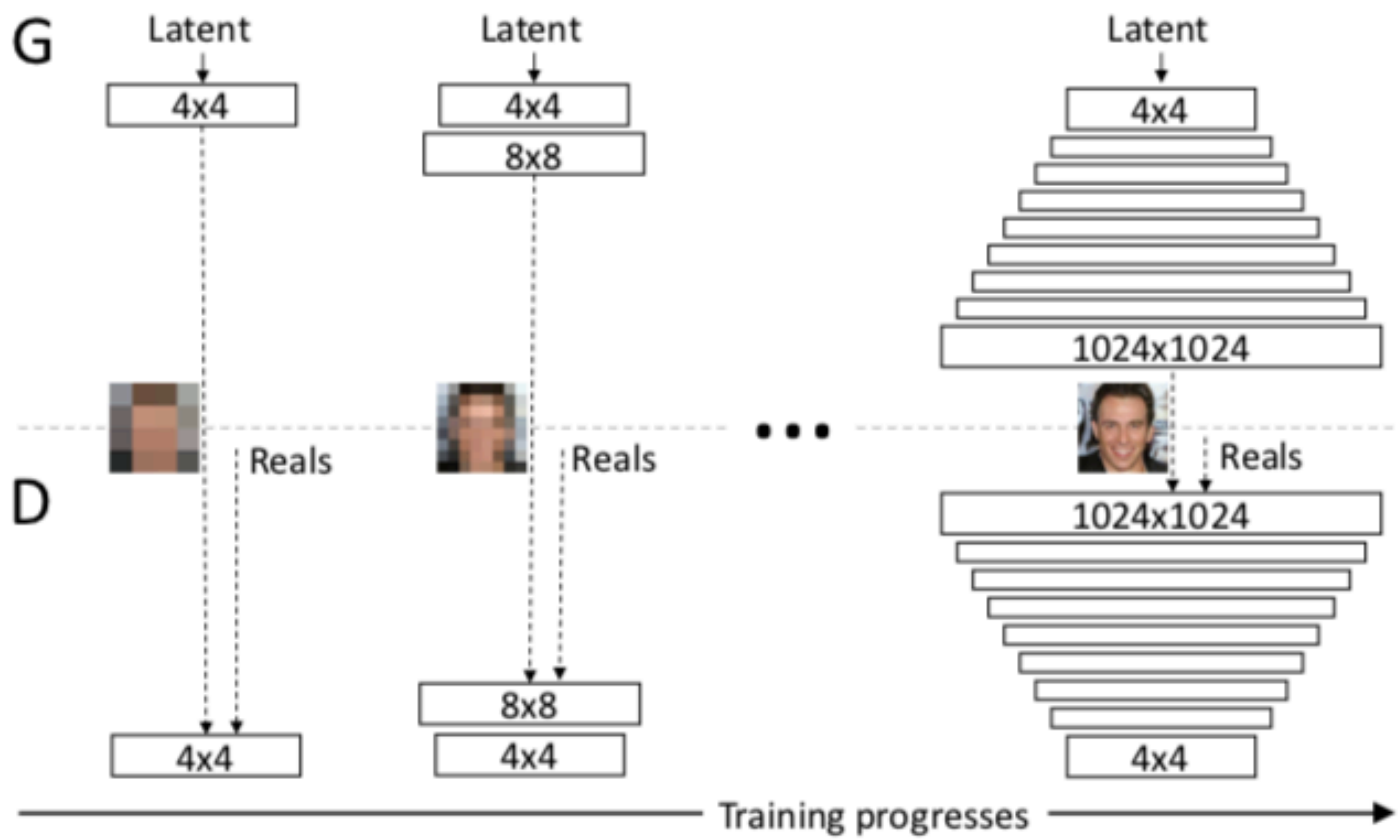
Considered structure

Key points

- Microstructures have stochastic nature and can be viewed as a realisation of a random variable
- Multiscale modelling techniques are widely used for microstructures:
  - for modelling the response and life prediction of composite materials (C.Oskay, 2015)
  - for flow estimation in porous media (Ronaldo Giro, 2018)
  - for modelling of crack propagation in random heterogeneous media (Darith−Anthony Hun et al., 2019)

Style-GAN

- Number of layers increases during training
- Maximal resolution on the train set - 256x256



StyleGAN architecture

Progressive Growing of GANs for Improved Quality, Stability, and Variation

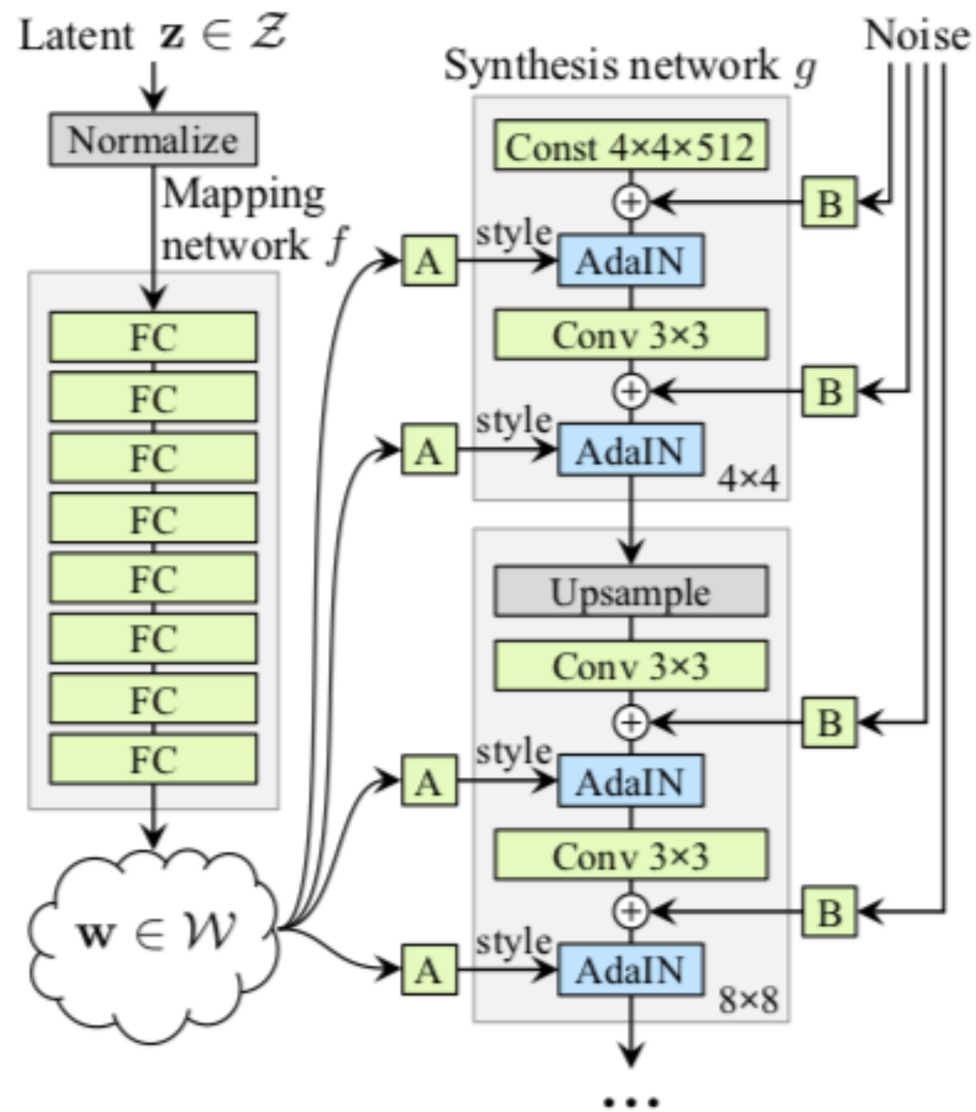
Style-GAN

- Style feature y for AdaIN operation:

$$\text{AdaIN}(x_i, y) = y_{s,i}\frac{x_i - \mu(x_i)}{\sigma(x_i)} + y_{b,i}$$

- Size of the output is equal to the size of train images

- Increase of size via image quilting



StyleGAN generator scheme
A - affine transform,
B - per-channel scaling of noise

A Style-Based Generator Architecture for Generative Adversarial Networks

Image quilting

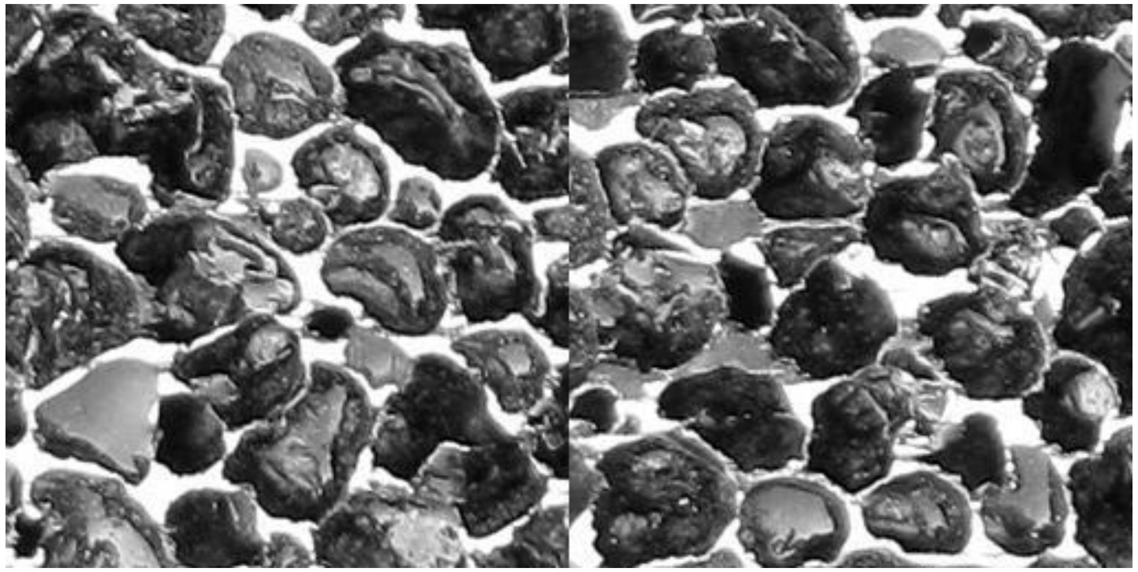


Image stacking without quilting

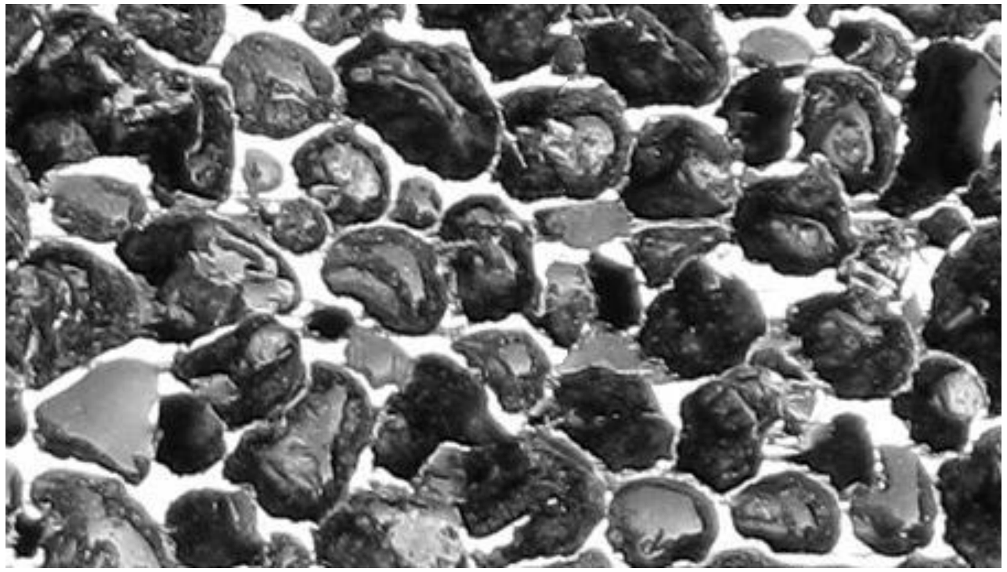
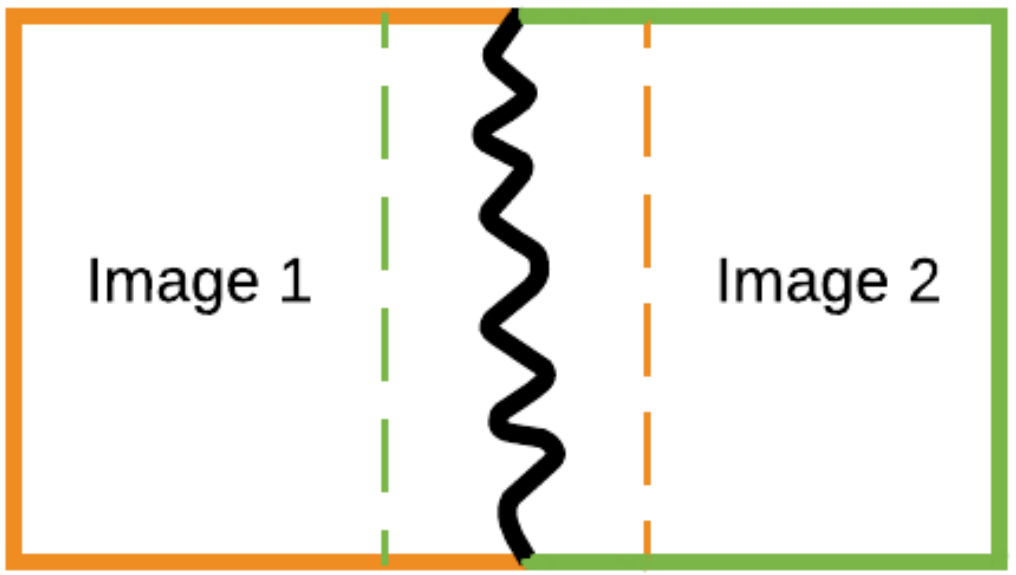


Image stacking with quilting

Image quilting

- Quilting paths - paths, minimising error on the overlap between two images
- Minimal error on (i,j)-th pixel of overlap:



Minimum boundary cut

$$E_{i,j} = \begin{cases} e_{i,j},\ j = 0 \\ e_{i,j} + min(E_{(i-1),j}; E_{(i-1),(j-1)}; E_{(i-1),(j+1)}), \text{ otherwise} \end{cases}$$

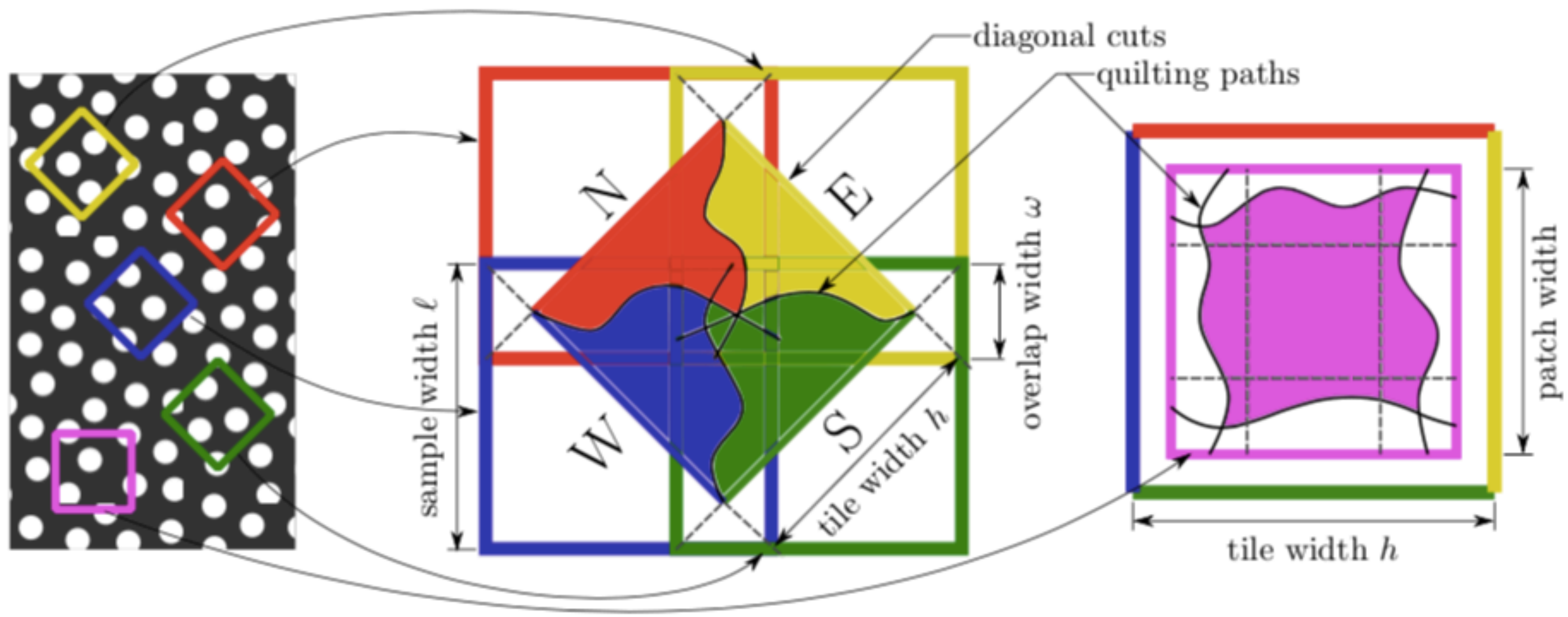
$e_{i,j} = (x_{i,j} - y_{i,j})^2$,

$x_{i,j}, y_{i,j}$ - (i,j)-th pixel of image 1

and 2 correspondingly

Wang tilings

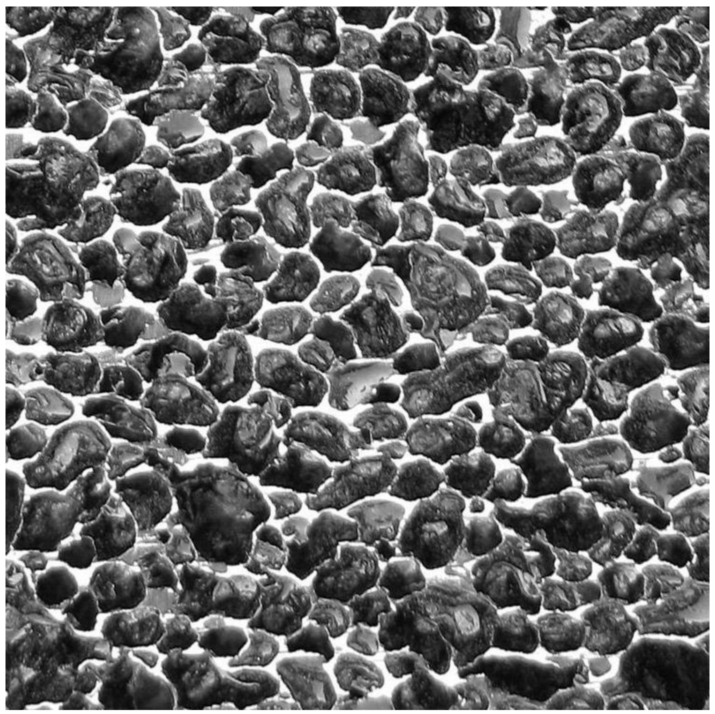
- The plane is covered with tilings chosen randomly from a set of 16 tilings with 4 colors of edges

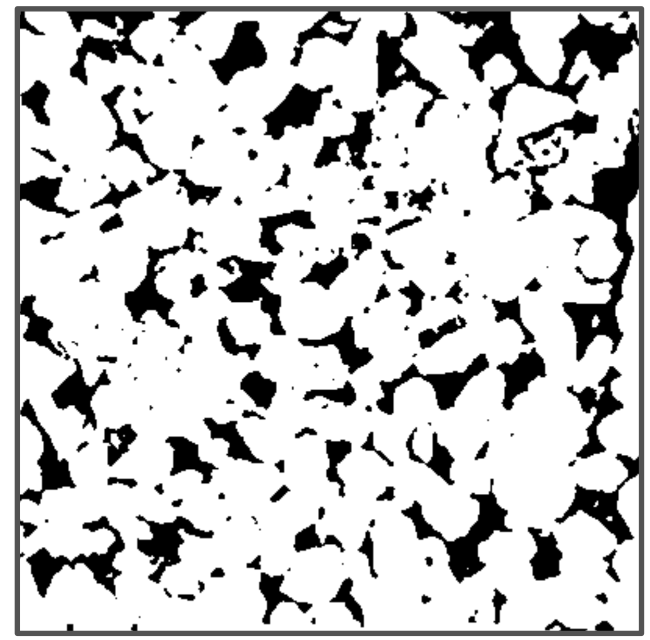


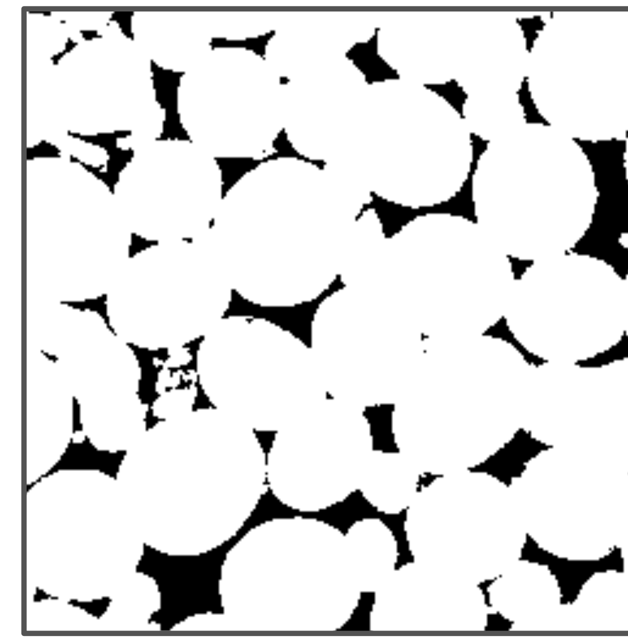
Process of tiles design

Experiments

Used structures


Alporas aluminium foam


Berea sandstone


Ketton limestone

Estimated values

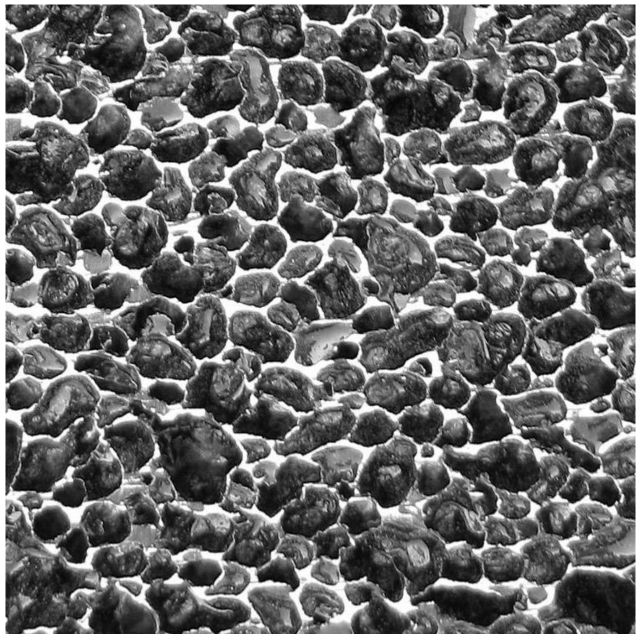
Mechanical properties

- Poisson's ratio (ν)
- Young's modulus (E)

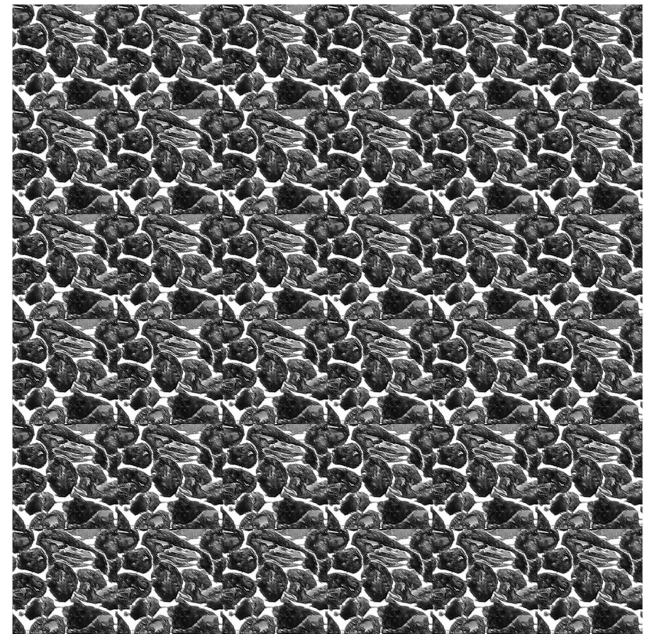
Minkowski functionals:

- Area density
- Perimeter density
- Euler2D density

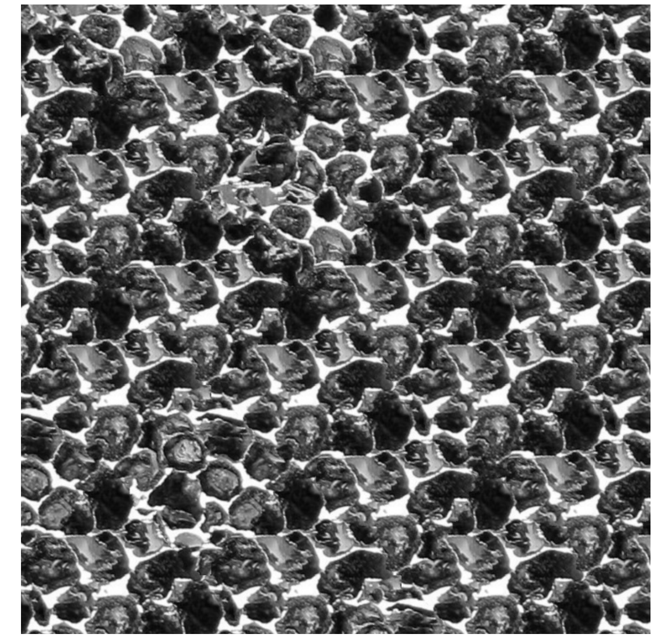
Visual comparison of the results



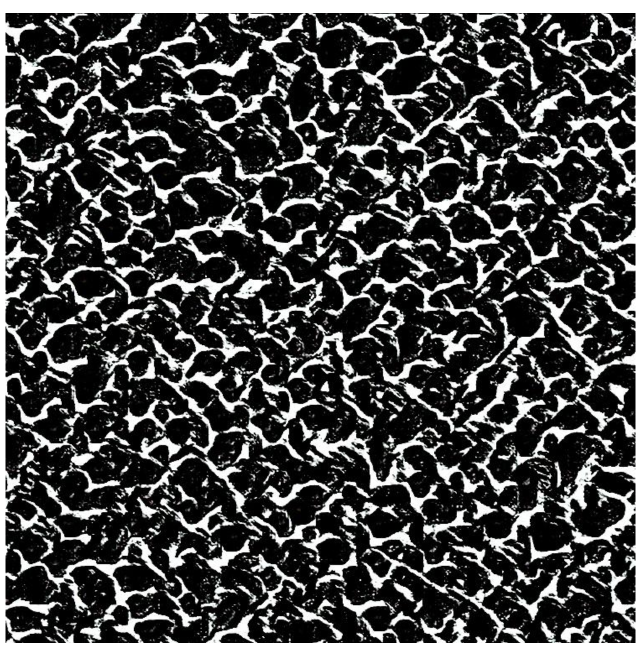
Original image



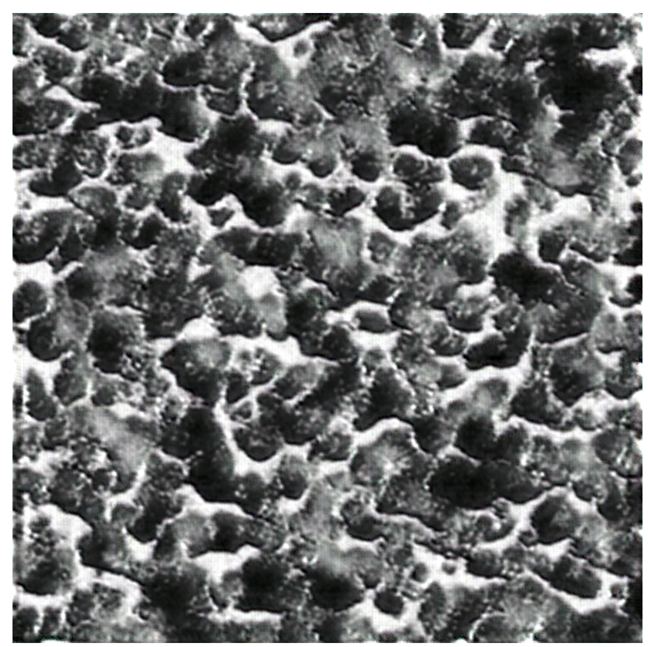
Periodic unit cell (PUC)



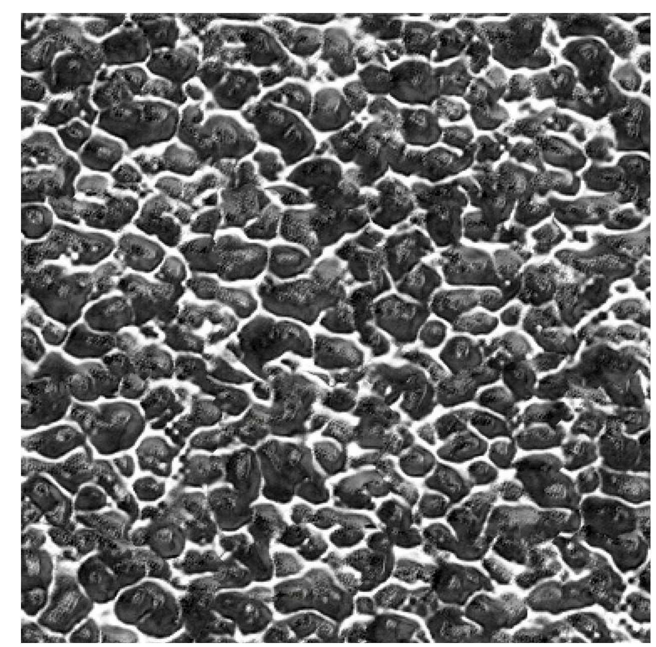
Wang tilings



Texture networks

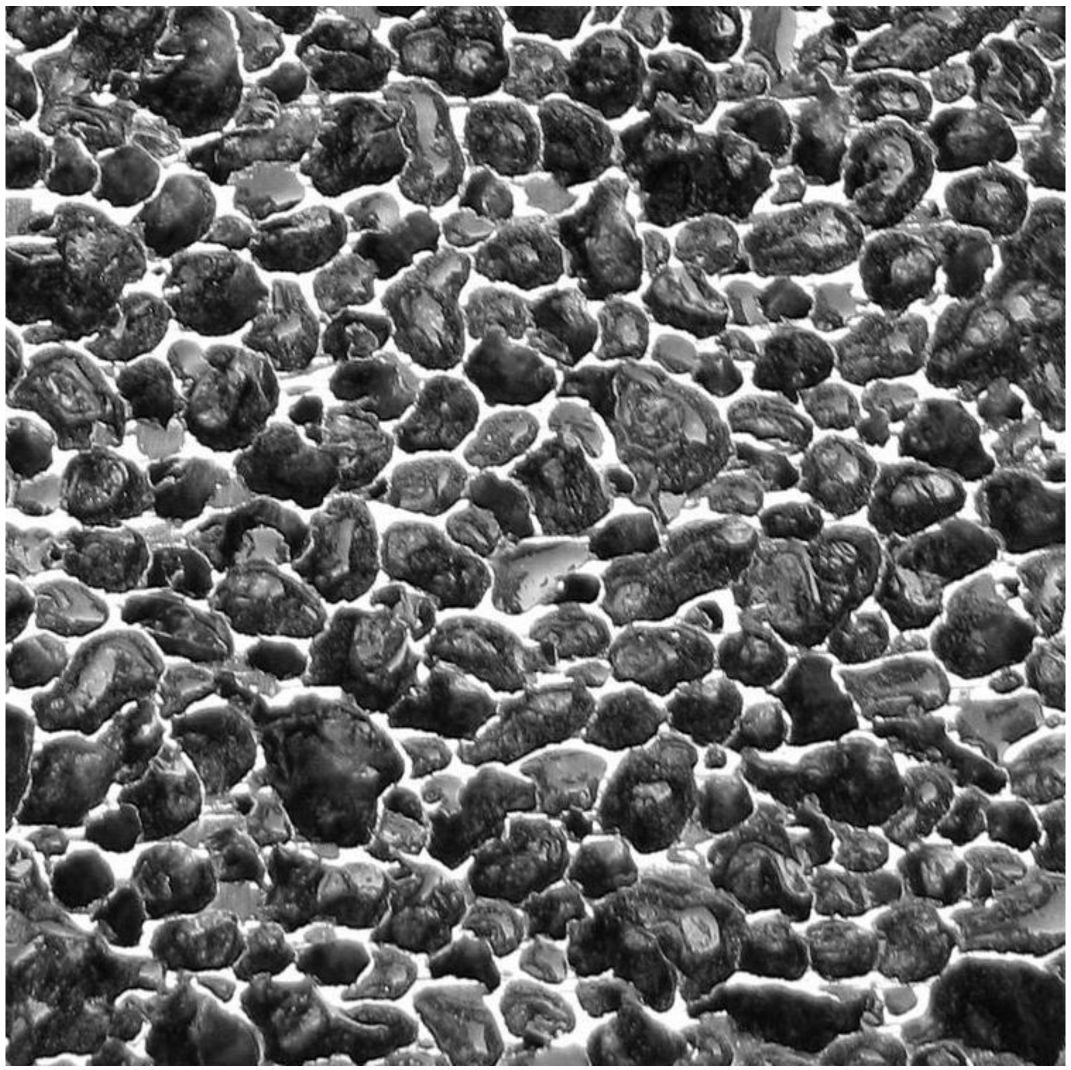


Spatial GAN

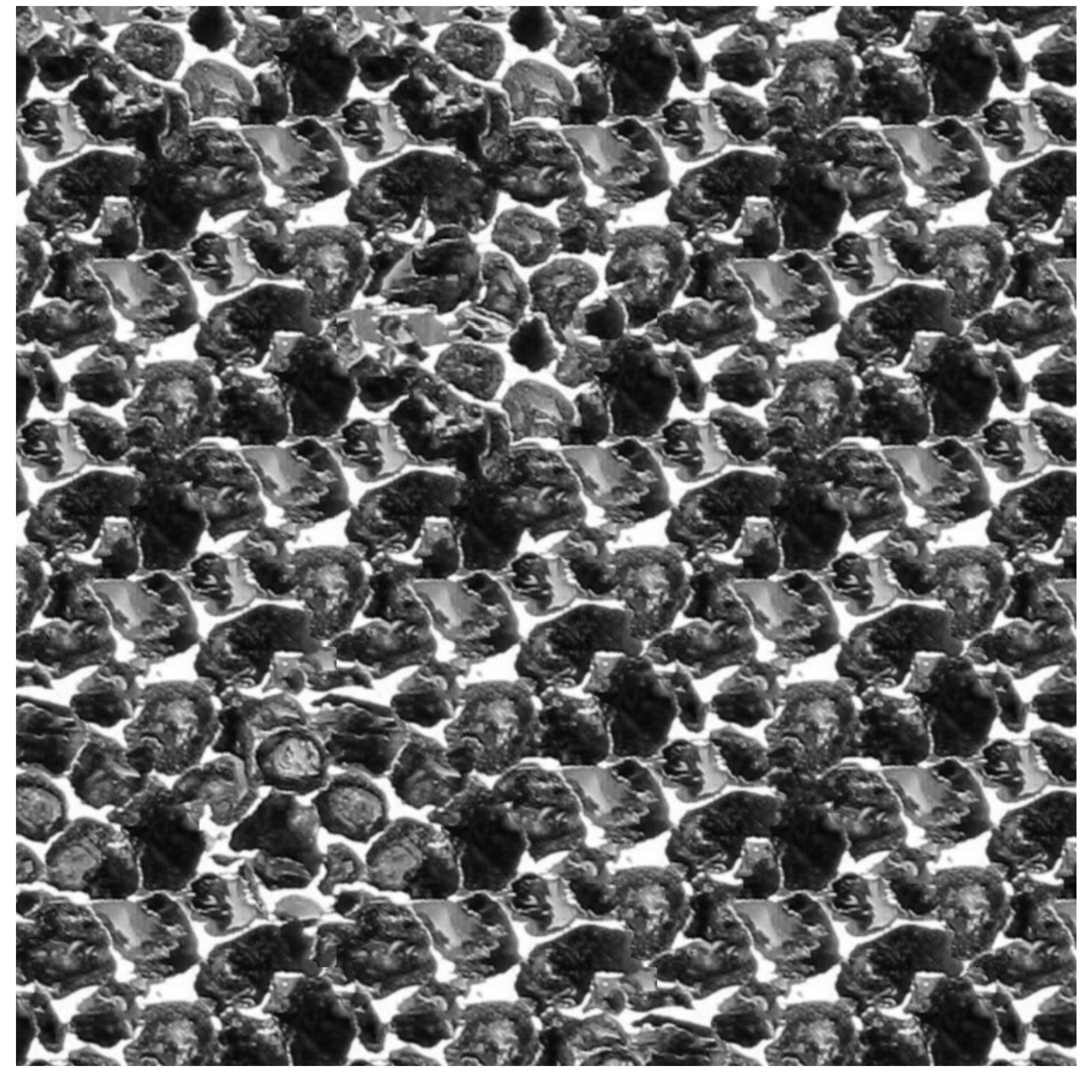


Style-GAN

Visual comparison of the results
Alporas

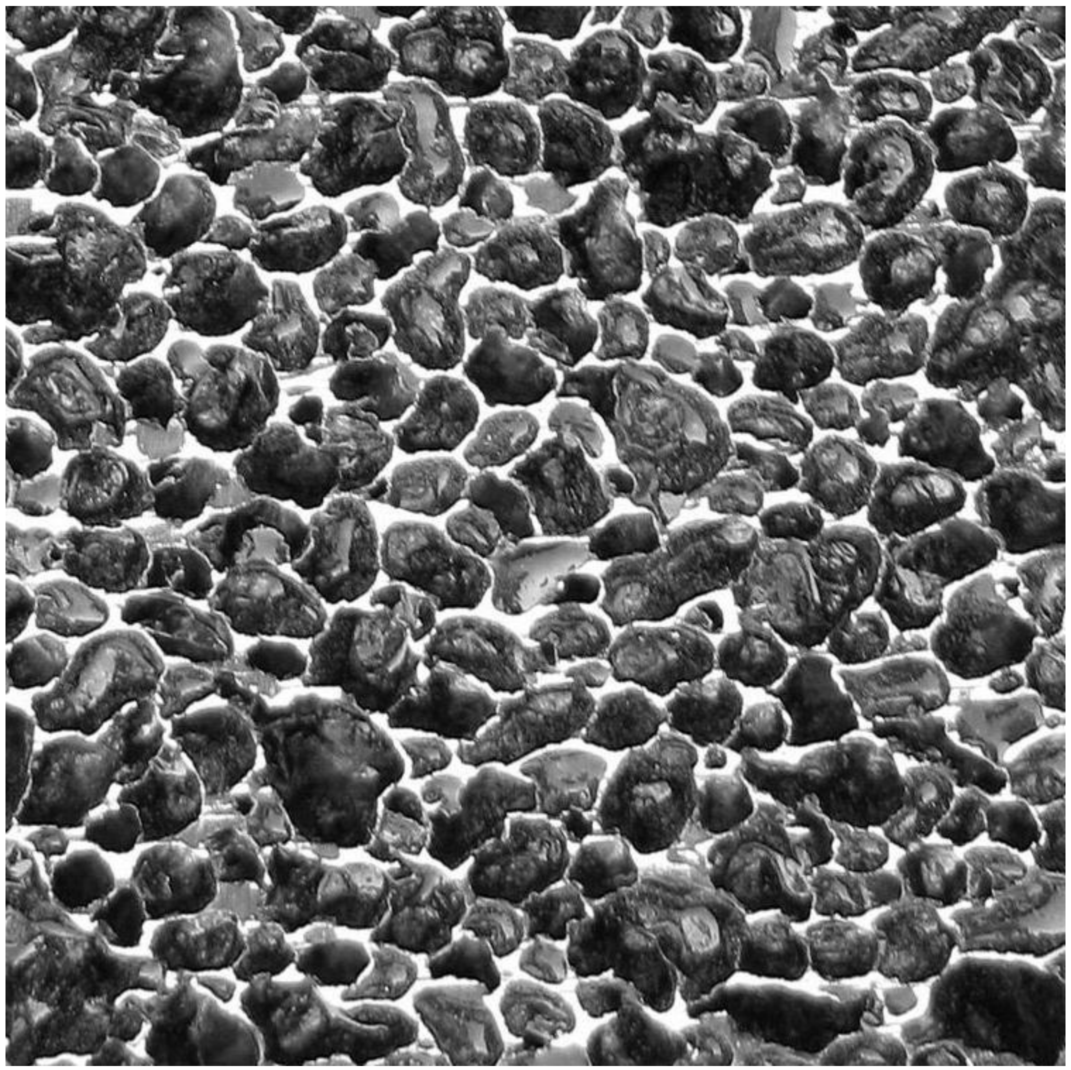


Original image

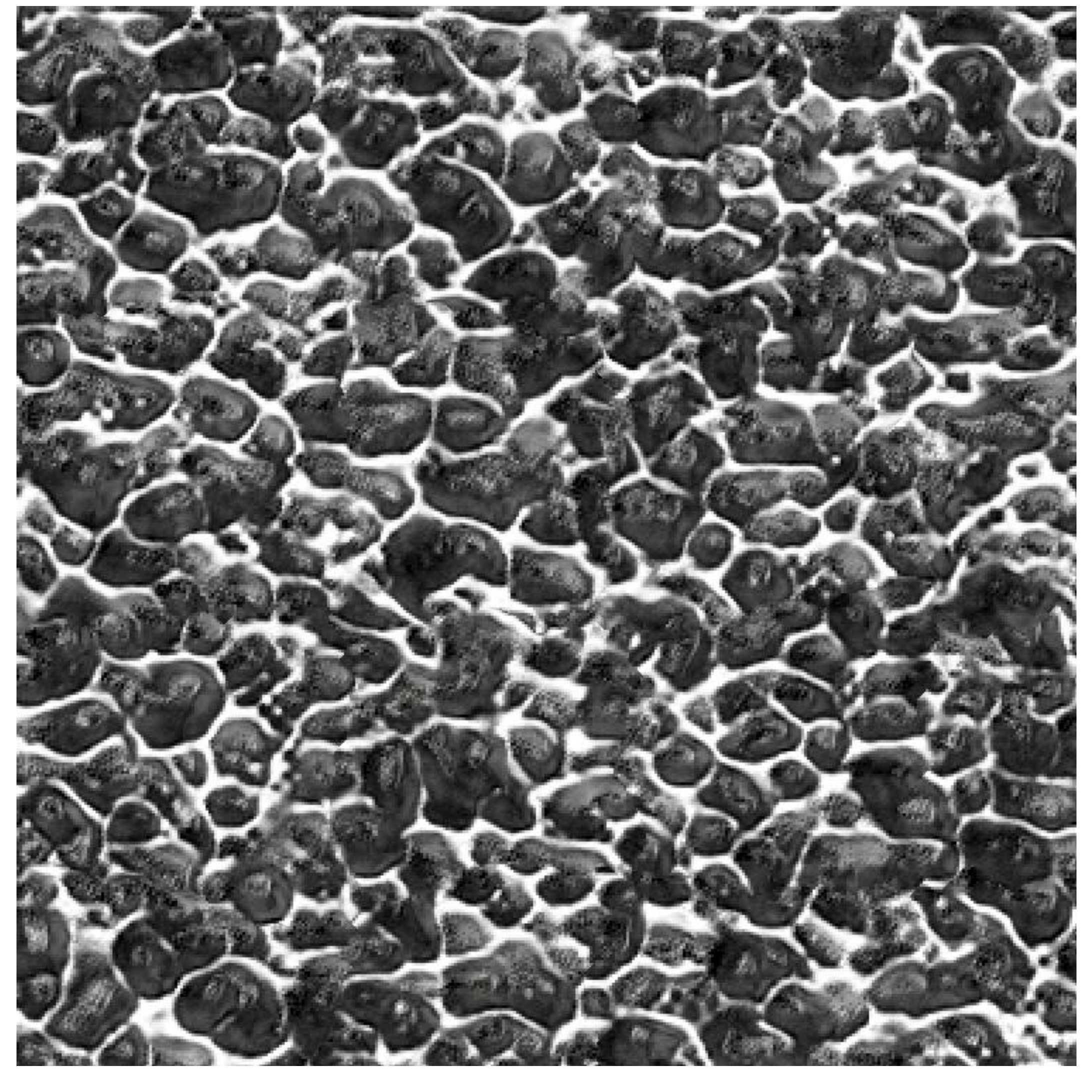


Wang tilings result

Visual comparison of the results
Alporas



Original image



Style-GAN result

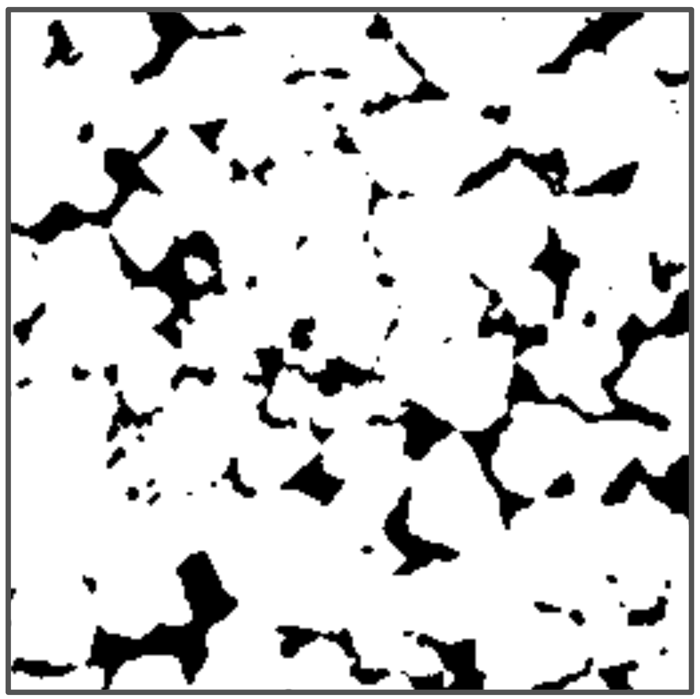
Numerical results
Mechanical properties

	Method		
	Original image	PUC	Wang tilings
E	0.0988 ± 0.0032	0.0966 ± 0.0112	0.0950 ± 0.0054
ν	0.3507 ± 0.0047	0.3460 ± 0.0190	0.3331 ± 0.0094

	Texture Networks	Spatial GAN	Style-GAN
E	0.0826 ± 0.0013	0.1120 ± 0.0094	$\mathbf{0.0958 \pm 0.0025}$
ν	0.3191 ± 0.0049	0.3266 ± 0.0129	$\mathbf{0.3634 \pm 0.0084}$

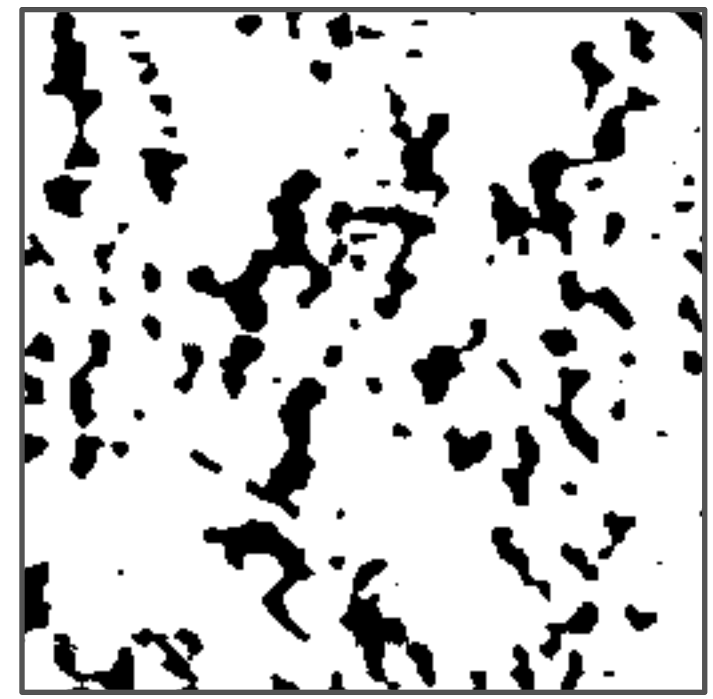
Visual comparison of the results

Berea



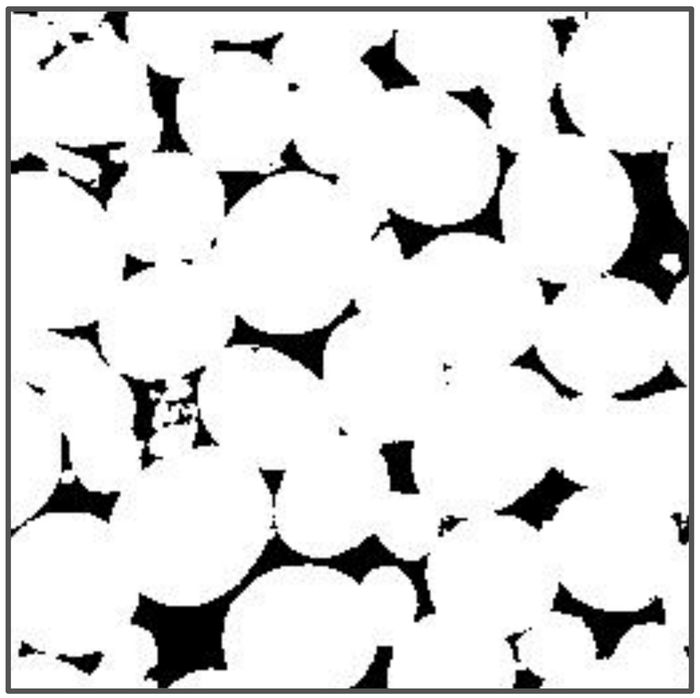
Original image

Wang tilings result



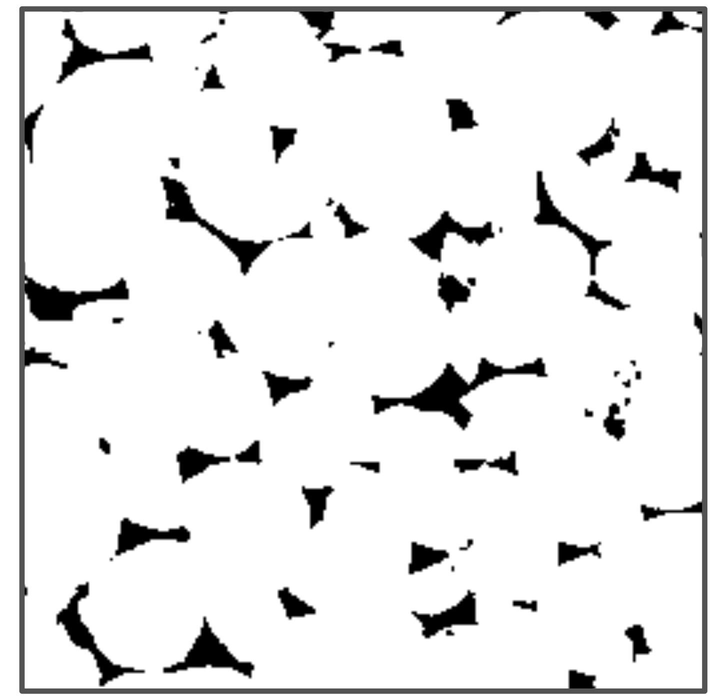
Style-GAN result

Visual comparison of the results
Ketton



Original image

Wang tilings result



Style-GAN result

Numerical results

Minkowski functionals

Berea

	Original image	Wang tilings	Style-GAN
Area	0.7970 ± 0.0528	0.8292 ± 0.0481	0.8167 ± 0.0046
Perimeter	0.0633 ± 0.0073	0.0653 ± 0.0115	0.0667 ± 0.0030
Euler2D	-0.0009 ± 0.0004	-0.0017 ± 0.0005	-0.0013 ± 0.0002

Ketton

	Original image	Wang tilings	Style-GAN
Area	0.8753 ± 0.0206	0.9149 ± 0.0323	0.9112 ± 0.0167
Perimeter	0.0501 ± 0.0054	0.0409 ± 0.0127	0.0438 ± 0.0059
Euler2D	-0.0008 ± 0.0003	-0.0010 ± 0.0004	-0.0011 ± 0.0003

Thank you for attention!

Appendix: Mechanical properties computation

Linear elastic equation

$$-\nabla(C^{base} : [\epsilon(w^{kl}) + e^{kl}]) = 0 \text{ in } Y,$$

where $\epsilon(w^{kl})$ is unknown strain tensor,

$$C^{base}\tau = 2\mu(\tau - \lambda \text{tr}(\tau) I) \cdot \rho, \;\; (C : \epsilon)_{ij} = \sum_{k,l} C_{ijkl}\epsilon_{kl},$$

$e^{kl} = \frac{1}{2}(e_k \otimes e_l + e_l \otimes e_k), \;\; e_k$ - column of identity matrix,

$\mu = E/(2(1 + nu)), \;\; \lambda = E\nu/(1 - \nu^2), \;\; E = 1.0, \nu = 0.3,$

ρ - material density

Appendix: Mechanical properties computation

Homogenised elasticity tensor:

$$C^H_{ijkl} = \frac{1}{|Y|} \int_\omega (e^{ij} + \epsilon(w^{ij}(y))) : C^{base} : (e^{ij} + \epsilon(w^{ij}(y)))dy$$

where:

$$C^{base}\tau = 2\mu(\tau - \lambda \mathrm{tr}(\tau)I) \cdot \rho,$$

$$\mu = E/(2(1+\nu)),\ \lambda = E\nu/(a - \nu^2),$$

$$E = 1.0,\ \nu = 0.3$$

Appendix: Minkowski functionals

Three functionals for two-dimensional structure:

- Area
- Perimeter
- Euler characteristic $\chi = V - E + F$, V - number of vertices,

E - number of edges, F - number of regions