Order parameter for images of structured arrays

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Sparse modelling and multi-exponential analysis,
Schloss Dagstuhl (DE), 14-19 June 2015

Summary

- Motivation
  honeycombs, nano arrays
- Image processing approach
- FFT approach & Problems

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Why is it not as simple as it seems?

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Bee honeycombs

- hexagonal wax cells
- 'perfect' = only few % deviation
- artificial comb
- irregular in transition worker-drone brood

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 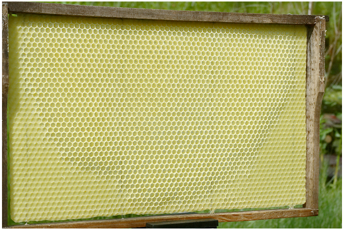

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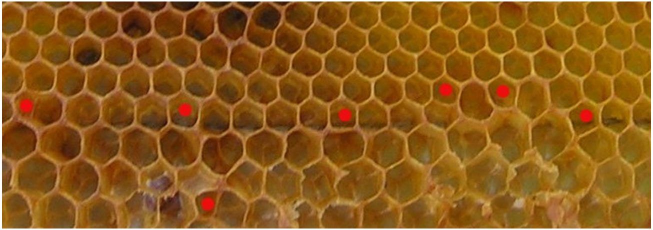

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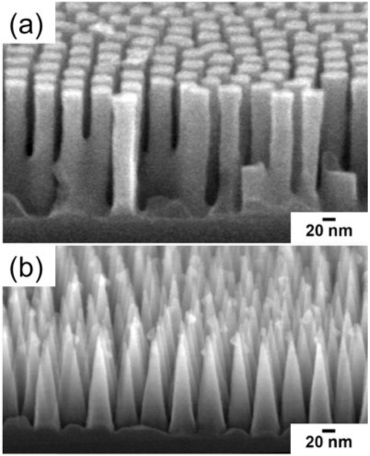
Nanopiles for hydrophobic surfaces



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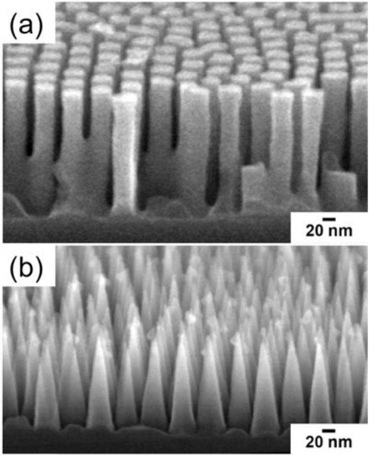

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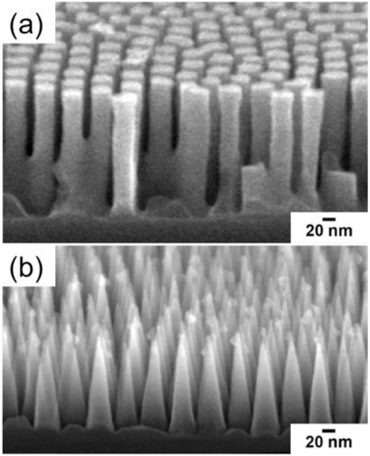

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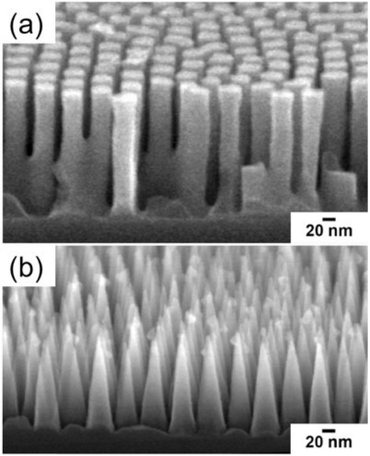
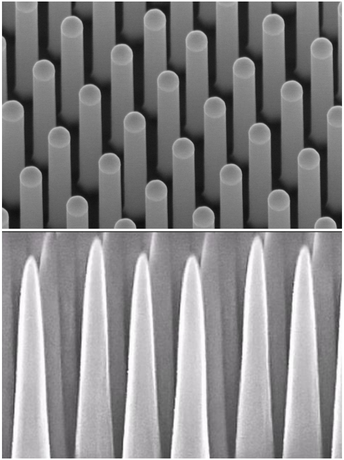
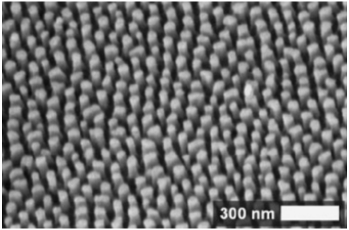
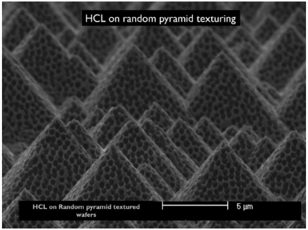




Nanowires and pyramids in solar cells





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- can be structured or not

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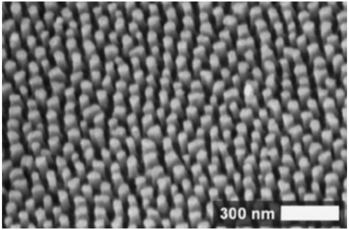

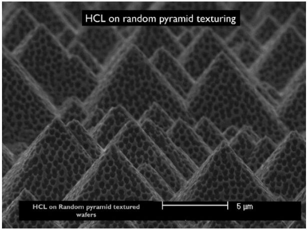

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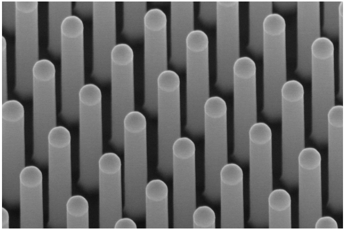
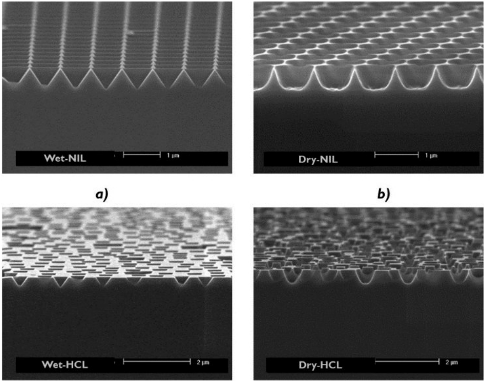
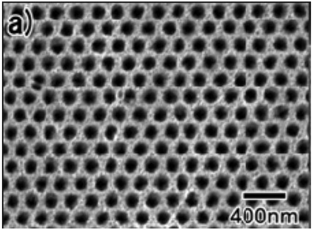




Nanopores in DNA analysis and biosensing



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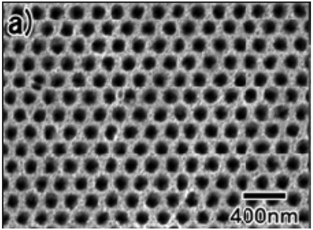

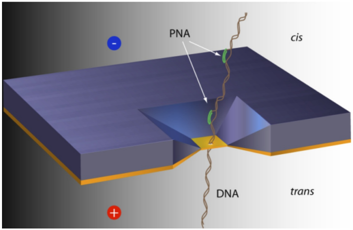

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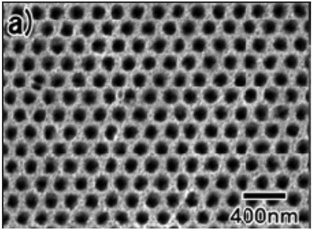

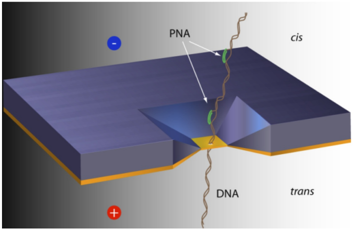

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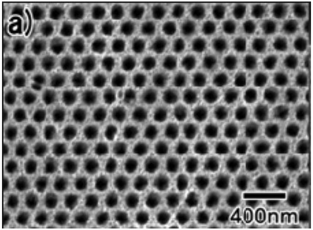

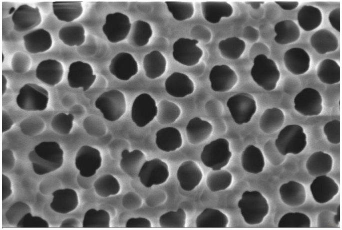

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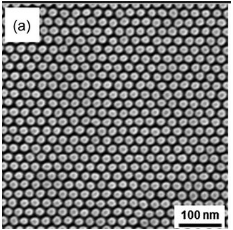
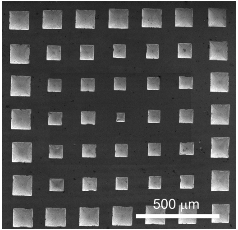
Several techniques for nanolithography

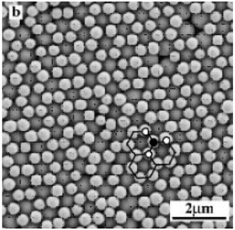
colloidal, plasmonic, nanosphere,... technologies used in nanolithography to produce several (regular) patterns at (micro or) nano scale



hexagonal



square



triangular

both in arrangement and/or in form of the grains

How much does it deviate from the perfect structure ?

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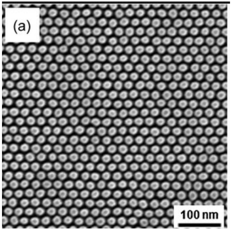

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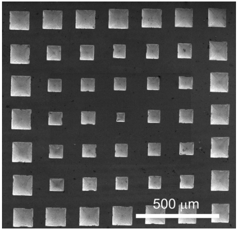

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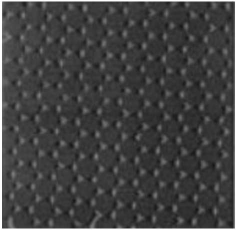

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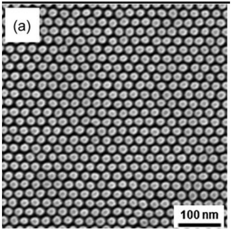

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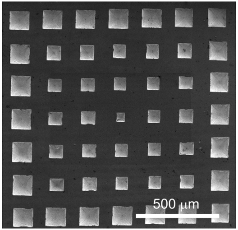

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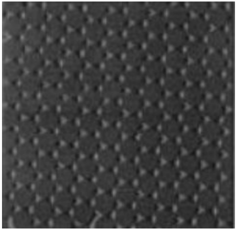

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Software (and companies) exist to do image analysis of pore images to compute e.g.

- diameter, max & min axis, centroid of pores
- statistics about the above and pore density
- ...

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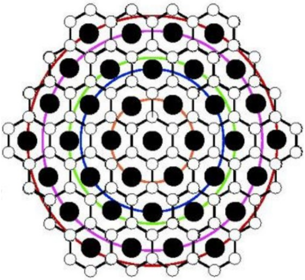
but that does not say much about the structure

Hexagonal topology



- nearest neighbor @ 1 (6 pores)
- next nearest neighbor @ $\sqrt{3}$ (6 pores)
- next nearest neighbor @ 2 (6 pores)
- next nearest neighbor @ $\sqrt{7}$ (12 pores)
- next nearest neighbor @ 3 (6 pores)
- ...

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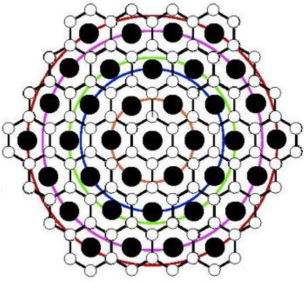

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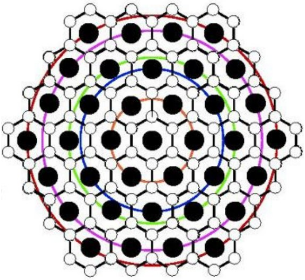

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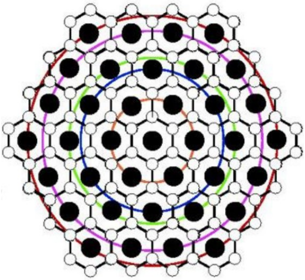

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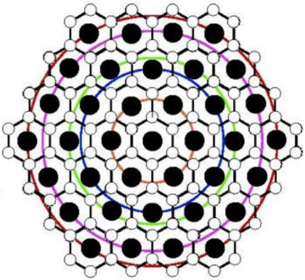

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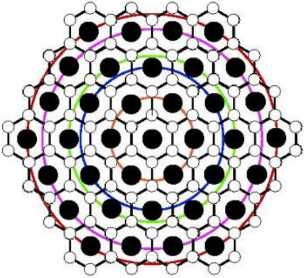

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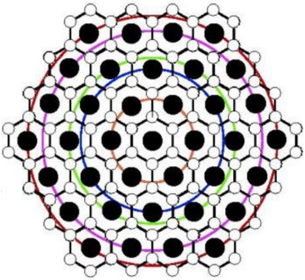

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Repeat for every pore and average $\Rightarrow$

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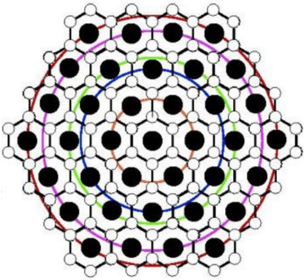

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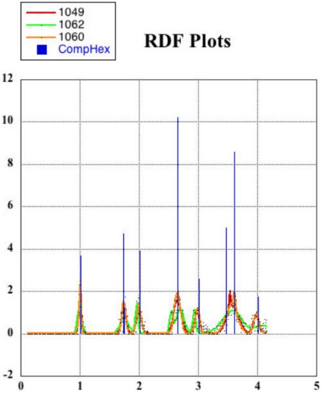
Non-perfect lattice: distributions with peaks at $1, \sqrt{3}, 2, \sqrt{7}, 3, \ldots$

Honeycomb examples

RDF of three honeycomb examples vs ideal RDF



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- Take out narrow part of the Gaussians at the ideal positions $\mathcal{P} = \{1, \sqrt{3}, 2, ..., 4\}$: $P = 3h\sum_{r\in\mathcal{P}} \rho(r)$
- compute the difference: $\Delta = T\rho - P$
- Use this to produce $OP_3 = 1 - \frac{\Delta}{T\rho} \in [0, 1]$,

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Kaatz,B,Egami, *Naturwissenschaften*, 2008

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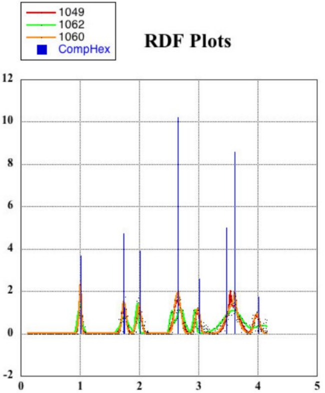

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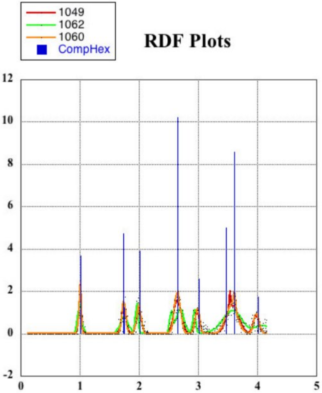

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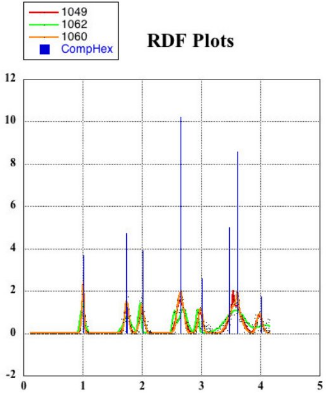

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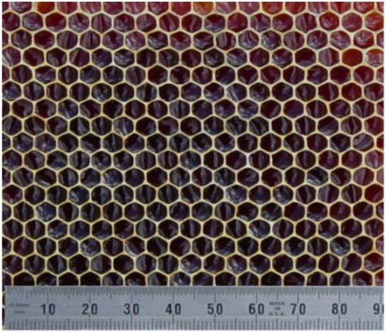
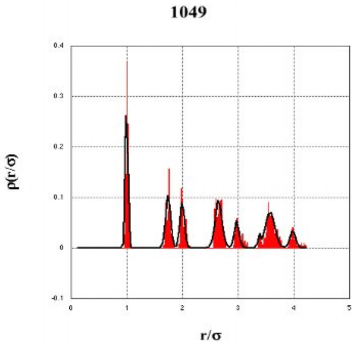
Bee comb example

One of the examples



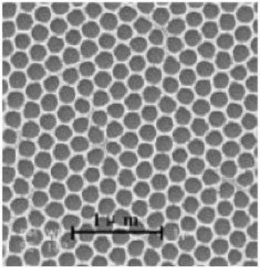


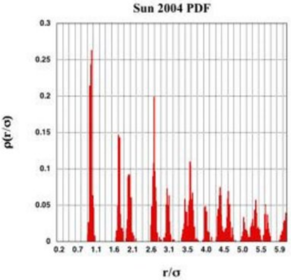
Pores and other arrays

What goes for hexagonal arrays goes for other arrays

hexagonal								
1	$\sqrt{3}$	2	$\sqrt{7}$	3	$\sqrt{12}$	$\sqrt{13}$	4	$\cdots$
6	6	6	12	6	6	12	6	$\cdots$
square								
1	$\sqrt{2}$	2	$\sqrt{5}$	$\sqrt{8}$	3	$\sqrt{10}$	$\sqrt{13}$	$\cdots$
4	4	4	8	4	4	8	8	$\cdots$
triangular								
1	$\sqrt{3}$	2	$\sqrt{7}$	3	$\sqrt{12}$	$\sqrt{13}$	4	$\cdots$
3	6	3	6	6	6	6	3	$\cdots$

Functional Material



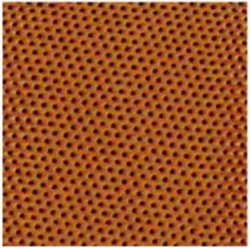


Sun 2004

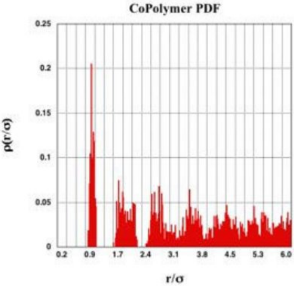
PDF $OP_3 = 0.598$

Kaatz,B,Egami, *J. Materials Science*, 2009

CoPolymers



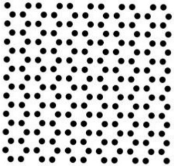
Kim 2004



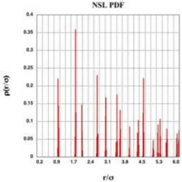
PDF $OP_3 = 0.242$

Kaatz,B,Egami, *J. Materials Science*, 2009

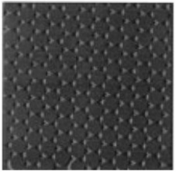
Nanosphere Lithography



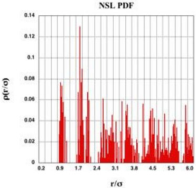
Ideal Array



$OP_3 = 0.906$



Hulteen 1999



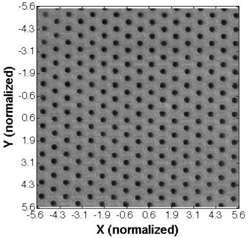
PDF $OP_3 = 0.267$

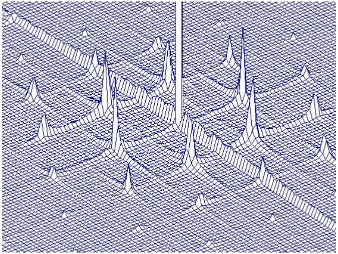
Kaatz,B,Egami, *J. Materials Science*, 2009

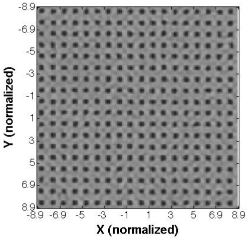
Summary

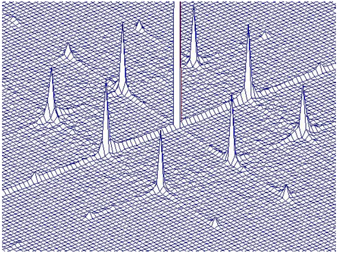
- Motivation
  honeycombs, nano arrays
- Image processing approach
- FFT approach & Problems

Take 2D FFT of the image









2D FFT

- Now get about the same info in 2D form for whole pic
- Don't need to repeat this for each pore
- Can we use the same technique?
- Here is what happens if the pores deviate from perfection

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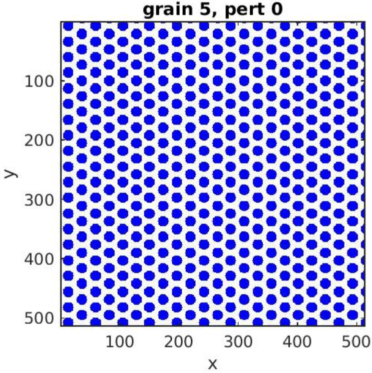
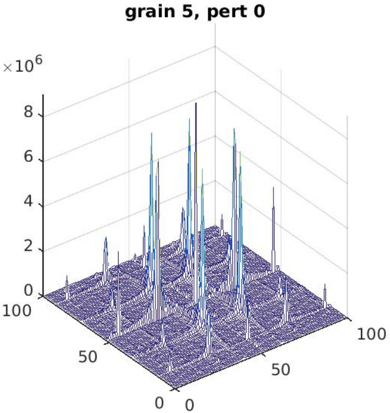
Hexagonal deviating from perfect

This is what happens as the pores deviate from a perfect array





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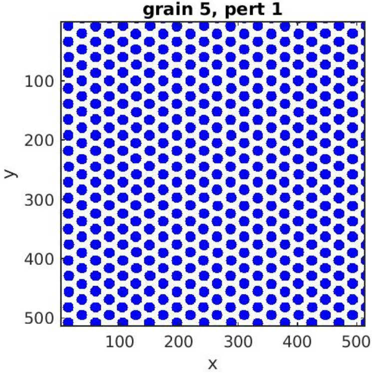

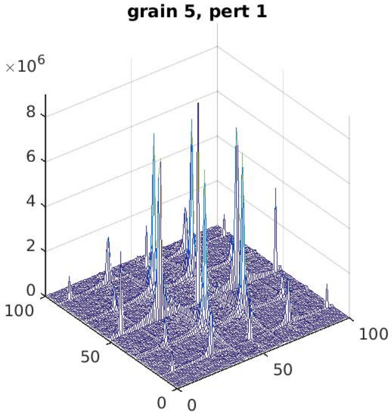

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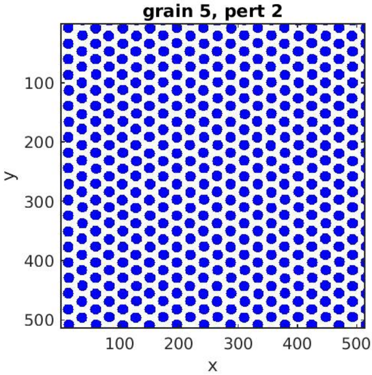

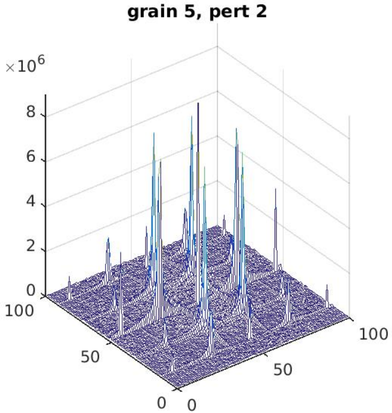

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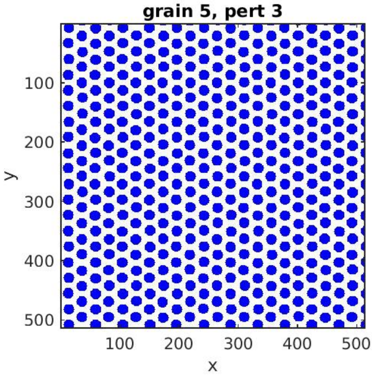

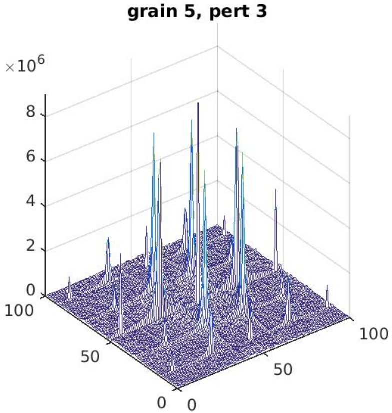

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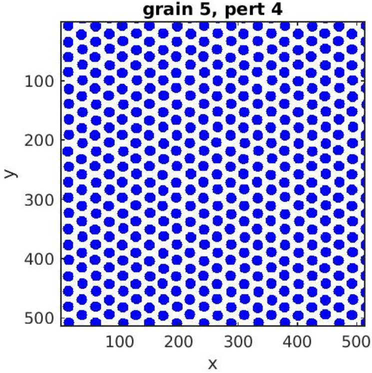

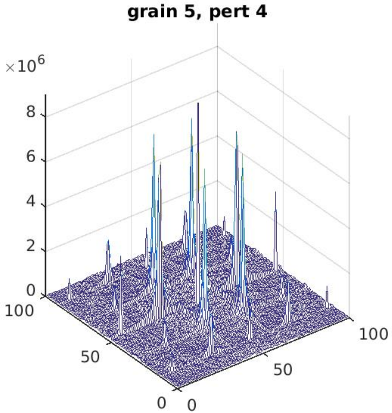

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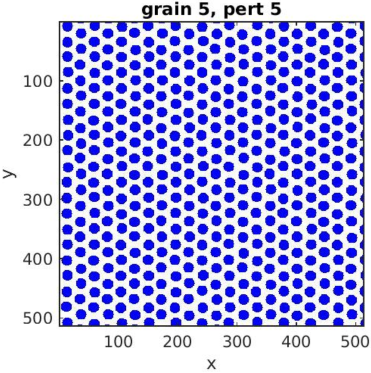

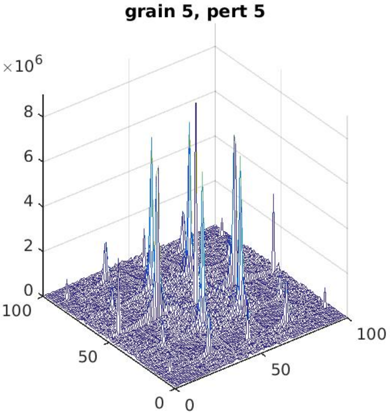

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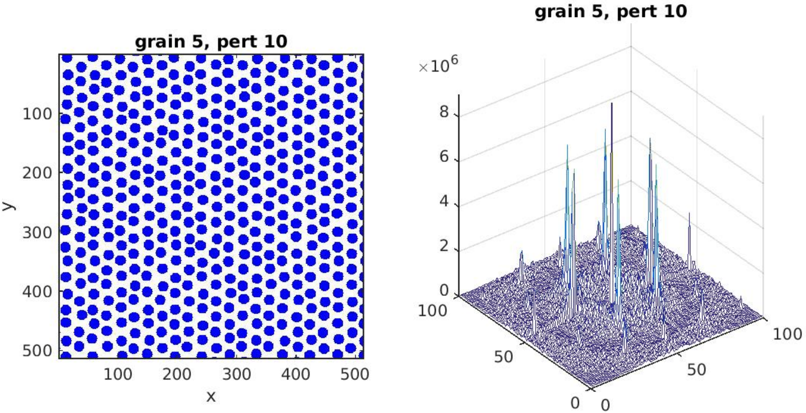

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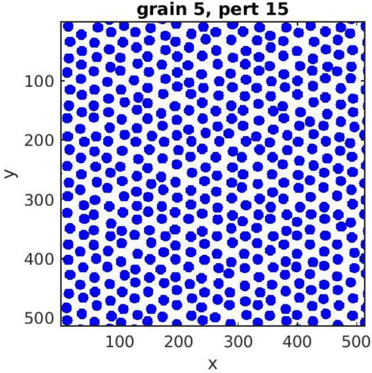

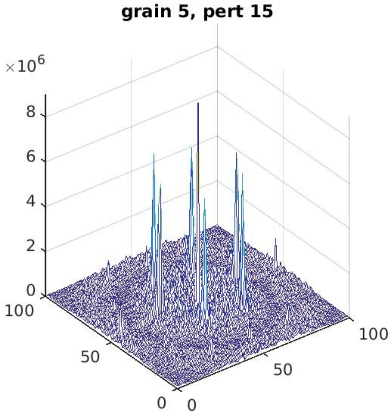

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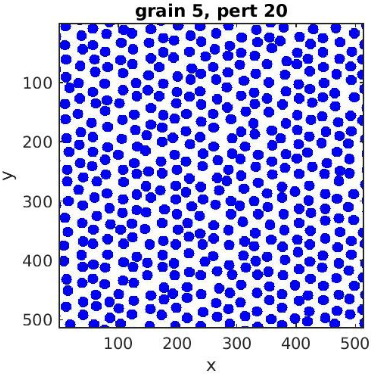

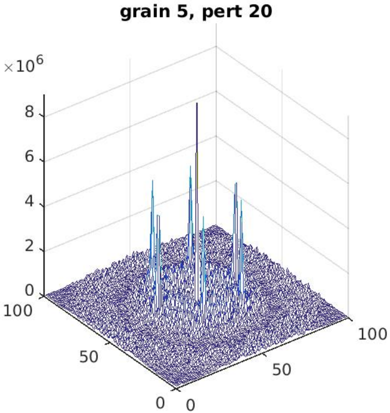

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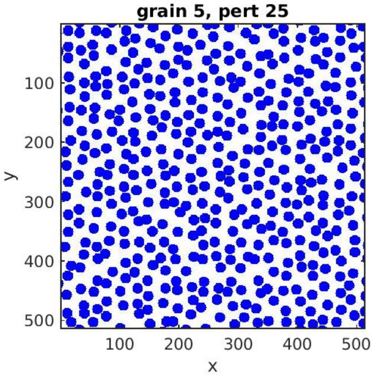

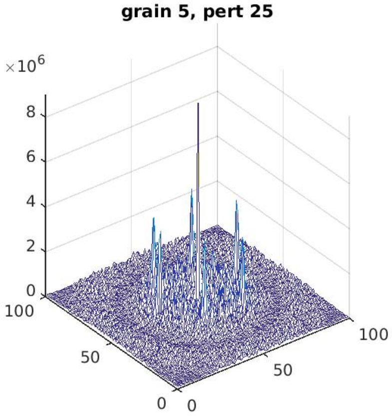

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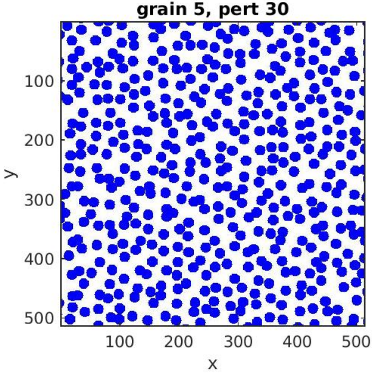
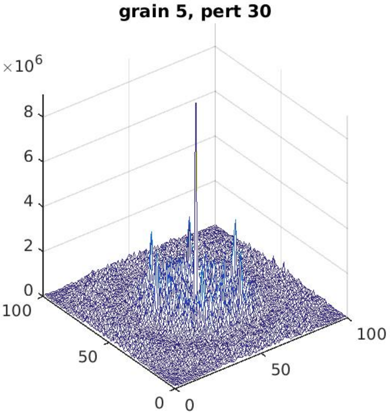
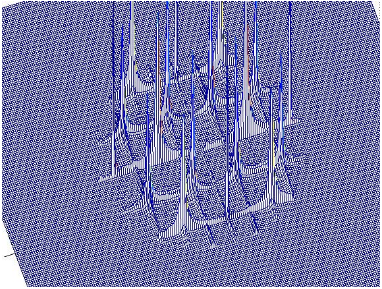




Radial distribution

- Consider only the central disk.
- Divide disk in concentric rings and compute average height/ring
- Surprise ...
- The x and y directions do not have the same scale for hexagonal
- After correction



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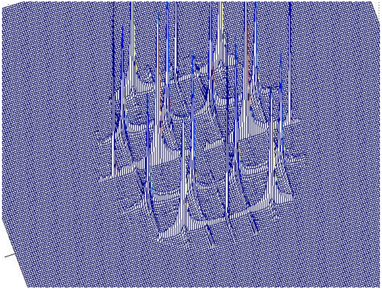

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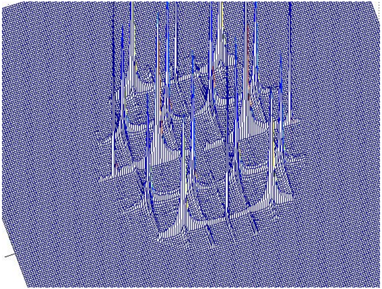

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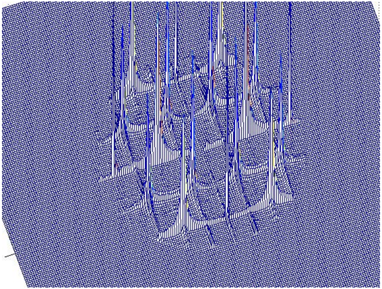

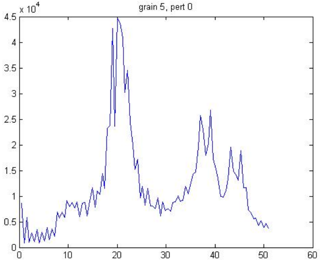

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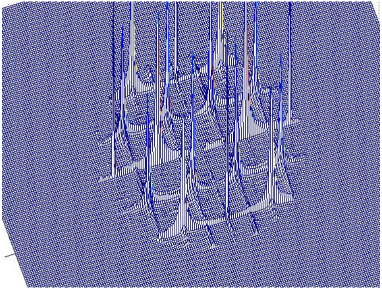
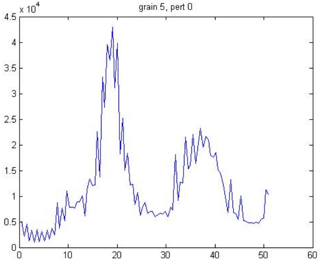
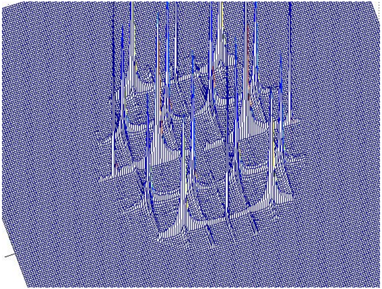
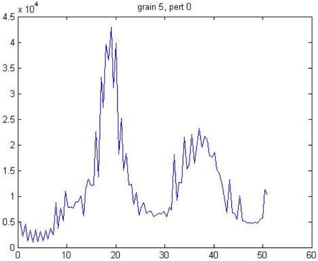




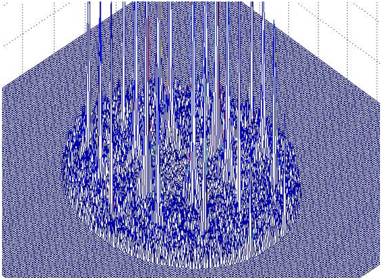
Radial distribution

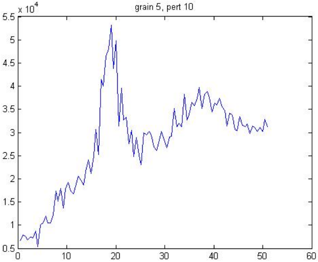
noiseless:





and after adding noise:





Radial distribution

However

- Fitting a sum of Gaussians is tricky
- The first peak is clear, the others are not so clear
- Consider only the peaks nearest to the center
- The ‘perfect’ images gives ‘more’ than peaks
- Look for an alternative
- Idea is: Peaks represent structure; the rest is noise
- How to identify peaks?

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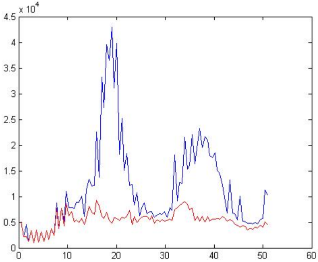
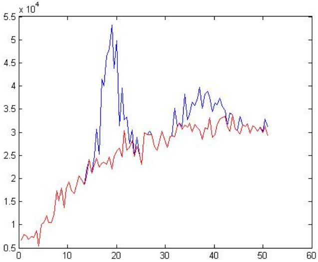
Radial distribution alternative

However

- Alternative = remove the peaks in 2D and recompute new average
  blue = with peaks, red = without peaks
  peak = anything sticking above 3 × average in 2D disk



no noise



noisy

- Take the ratio of the red integral (=sum) over the blue one
- Order Parameter OP = 1 - red/blue.
- In practice resolution is much lower

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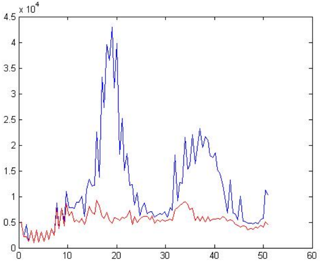

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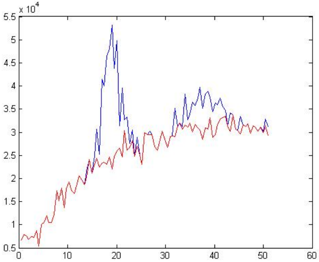

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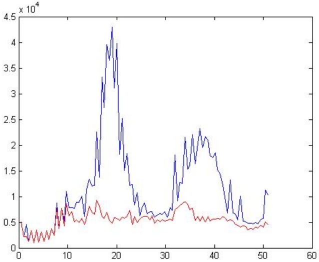

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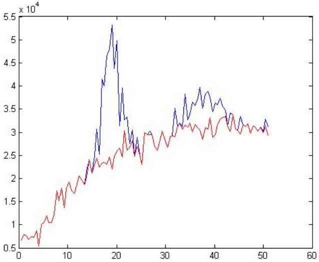

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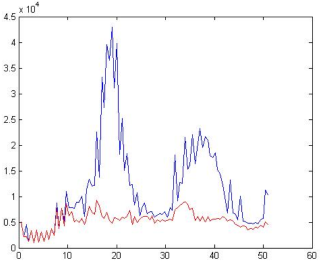

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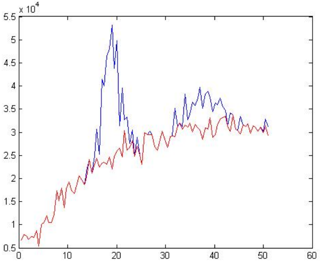

noisy

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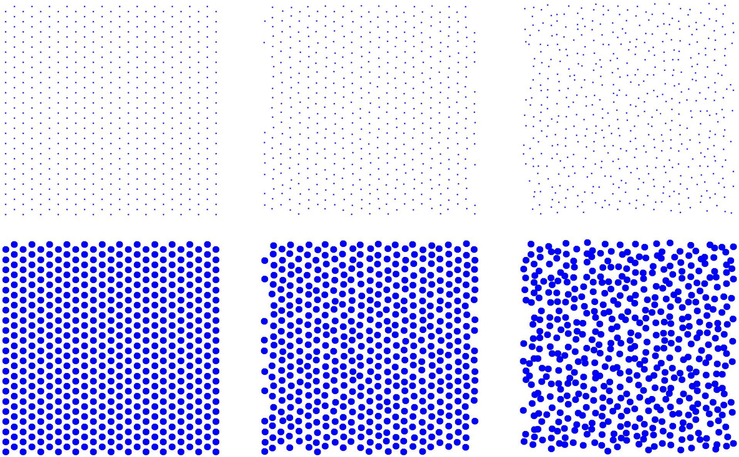
Radial distribution alternative

For different grain sizes and different perturbations

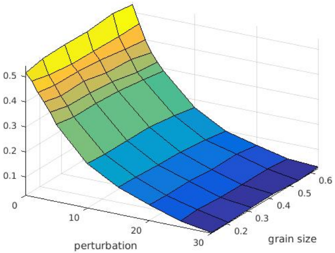
0% | 10% | 30%

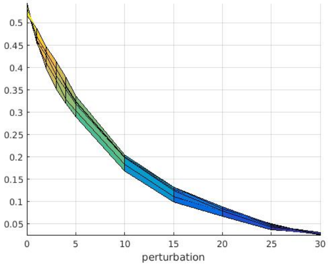


Radial distribution alternative

Hexagonal

- Repeat for different grain sizes and different perturbations



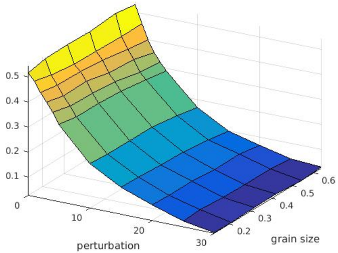


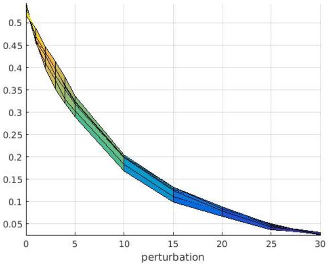
- Depends somewhat on grain size
- More reliable for small perturbations

Radial distribution alternative

Hexagonal

- Repeat for different grain sizes and different perturbations





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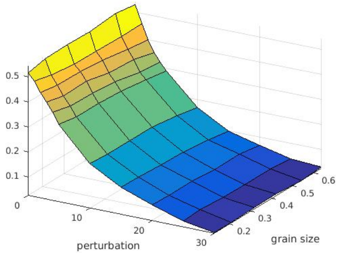

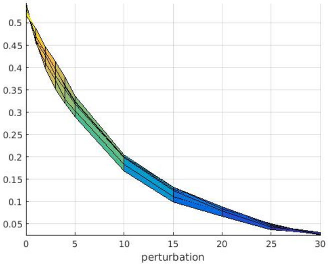

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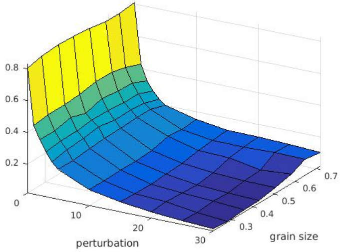
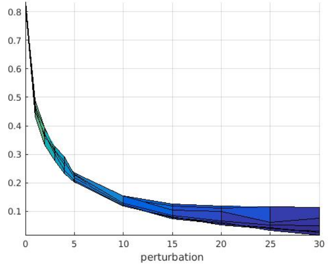
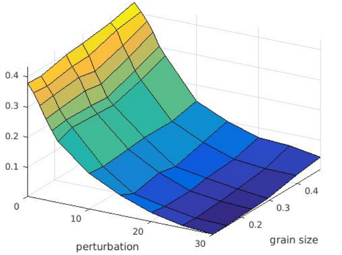
Radial distribution alternative

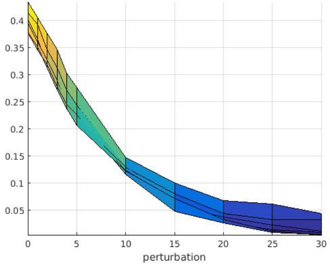
Square





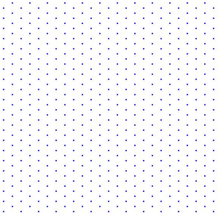
Triangular



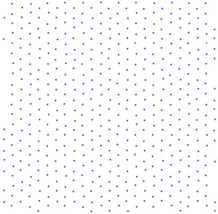


Radial distribution alternative

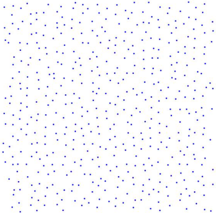
0% OP=0.5147



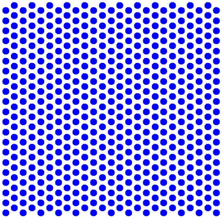
10% OP=0.2042



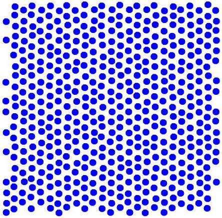
30% OP=0.0257



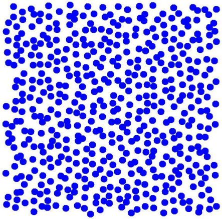
0% OP=0.5308



10% OP=0.1688

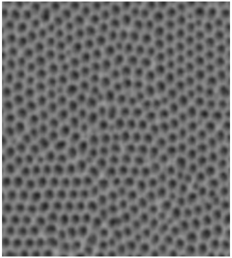


30% OP=0.0292



Example no structure

$\text{OP} = 0.08$

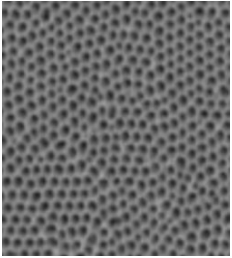


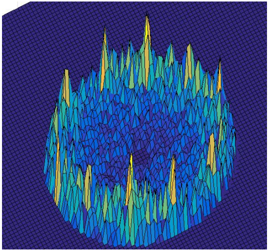
Peaks do not represent 4 or 6 directional structure.

Example is chaotic, but distance between centers is almost constant in all directions. Hence FFT looks like

Example no structure

OP $= 0.08$





Peaks do not represent 4 or 6 directional structure.

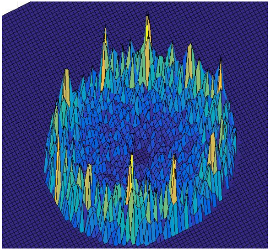
Example is chaotic, but distance between centers is almost constant in all directions. Hence FFT looks like

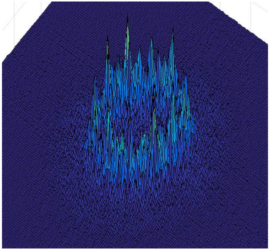
hence much energy comes from the peaks again.

Example no structure

The selection of the disk is very important

OP $= 0.08/0.01$ OP $= 0.58$





If the disk is larger, then more small values enter.
Hence the average is smaller.
'By definition': peak $=$ higher than 3 $\times$ average
Hence remove also many high values that are not isolated peaks.
Thus all energy comes from the 'peaks' $=$ highly structured.

Two strategies

What is defined to be a peak?

Either take average over disk and define peak everything in the disk that is higher than $3 \times$ the average.

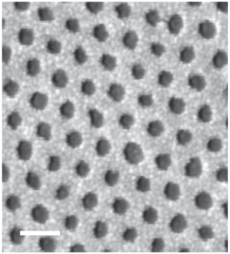
Or divide disk into concentric rings en compute per ring the average and define peak within that ring as everything higher than $3 \times$ the average over that ring

Then def peak, hence OP less depending on the size of the disk.

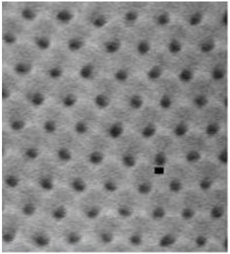
Two OP values: depending on disk avg or ring avg.

Practical examples

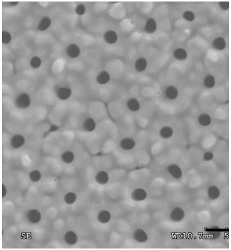
OP=0.23/0.18



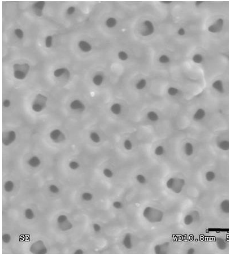
OP=0.19/0.23



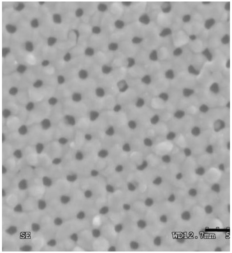
OP=0.15/0.06



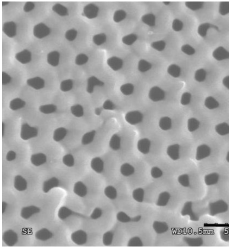
OP=0.09/0.05



OP=0.14/0.12

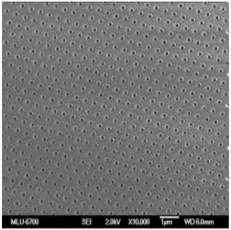


OP=0.14/0.11

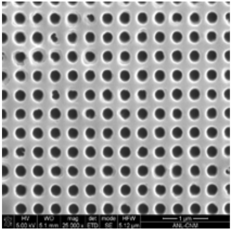


Practical examples

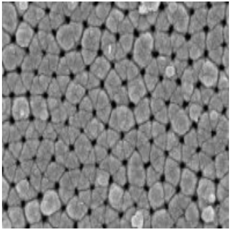
OP=0.49/0.36



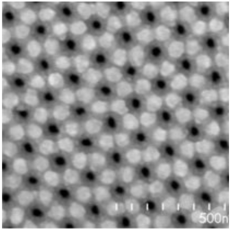
OP=0.14/0.11



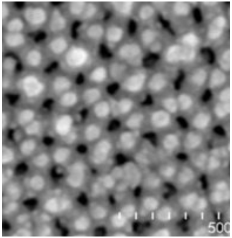
OP=0.02/0.00



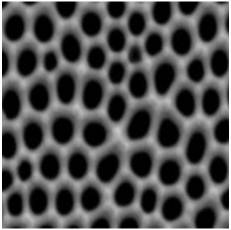
OP=0.27/0.29



OP=0.03/0.02

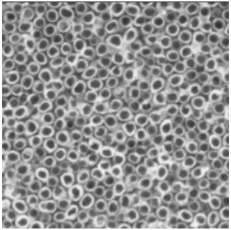


OP=0.07/0.02

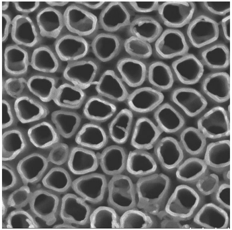


Not structured examples

OP=0.00/0.00



OP=0.05/0.01



Radial distribution alternative

Still problems: requires fine tuning

- Depends on form of the grains and grain size
- All grains assumed same size and all disks
- Very sensitive to selection of the relevant disk in FFT plane
  - ▷ nearest peaks radius depends on distance between grain centers
  - ▷ averages over disk/ring define what is a peak
  - ▷ hence what is structure and what is not, hence the OP
- Unreliable when peaks drown in noise peaks
- Does not really detect 4 or 6-fold symmetry
- Small variation depending on resolution of radial distributions
- ...

There is some potential for comparing a set of similar images with small perturbations

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