Influence of polydispersity on the structure of colloidal crystals revealed by X-ray diffraction

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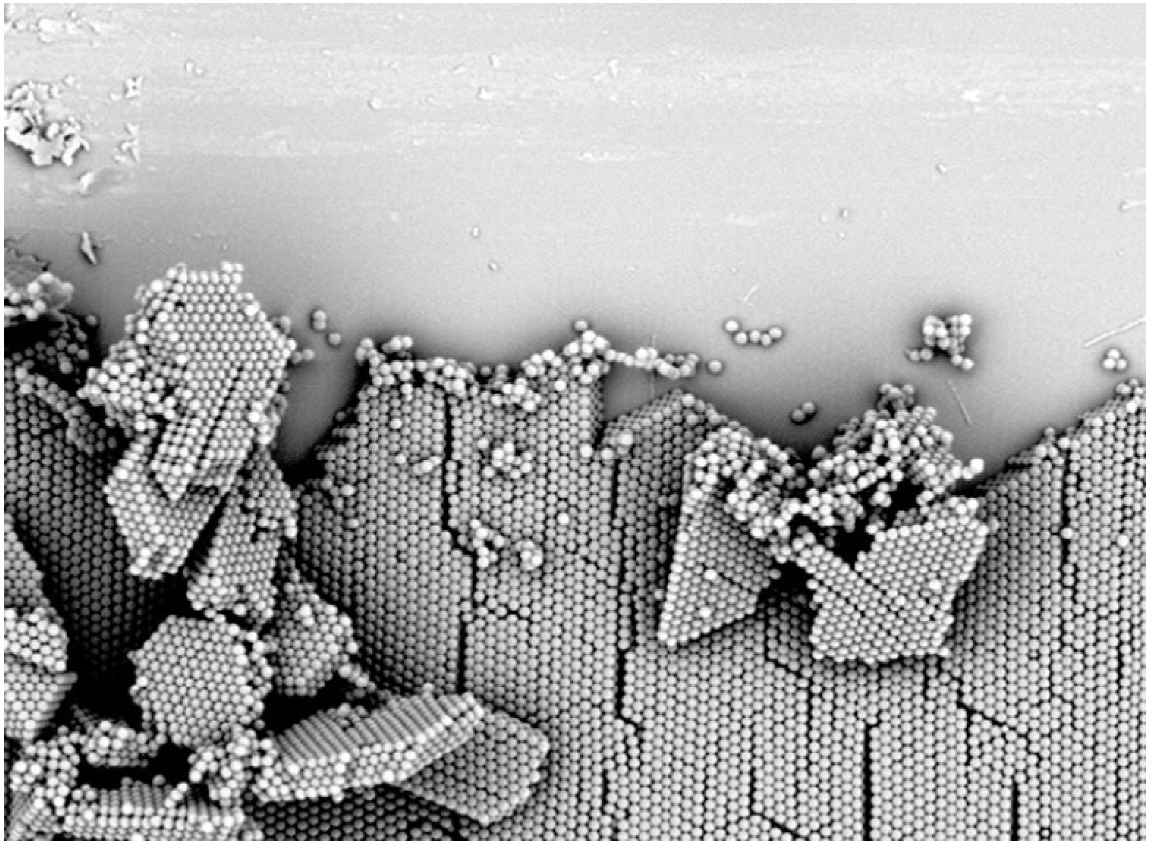
Colloidal structures

Typical size: from 1 to 1000 nanometers. Different colors are caused by polydispersity.

Colloidal crystals in nature.

Colloidal structures

These crystals are used as photonic band gap materials – *photonic crystals*.
Dispersion of particle radius has influence on crystal structure.



SEM image of a colloidal crystal film.

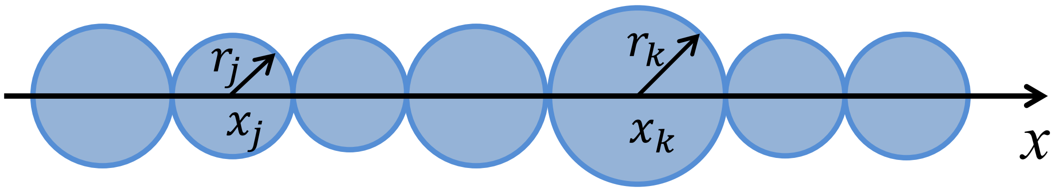
Jahne-Mieke Meijer. PhD Thesis.

Project aims

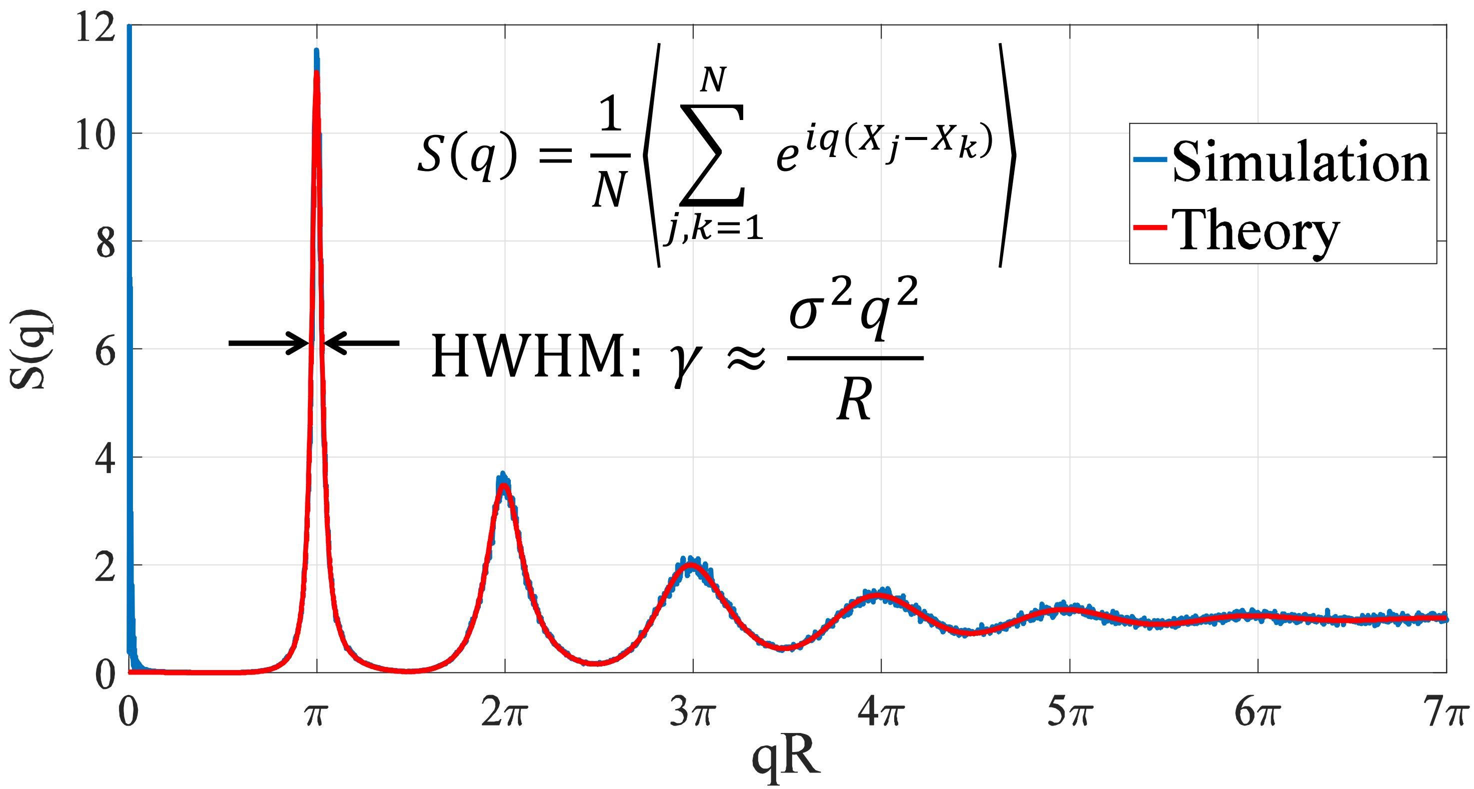
- generate two dimensional colloidal crystal lattice
- calculate X-ray diffraction pattern
- analyze dispersion of particle radius influence on Bragg peak width

One-dimensional case

Theory and simulation by I.Zaluzhnyy

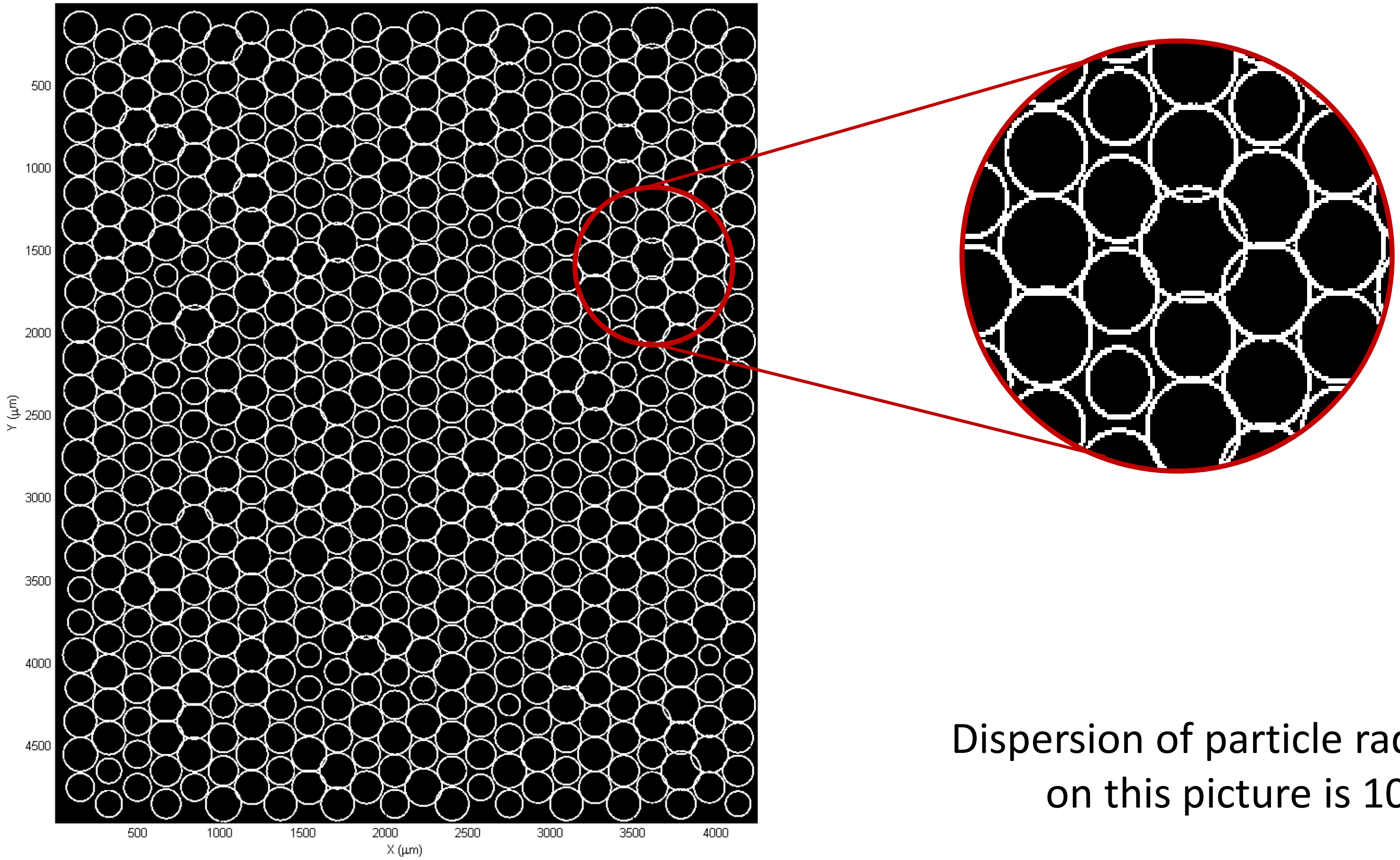


$$\begin{cases} x_1 = 0 \\ x_{j+1} - x_j = r_{j+1} + r_j \\ r_j \sim N(R, \sigma^2) \end{cases}$$



Ideal hexagonal lattice

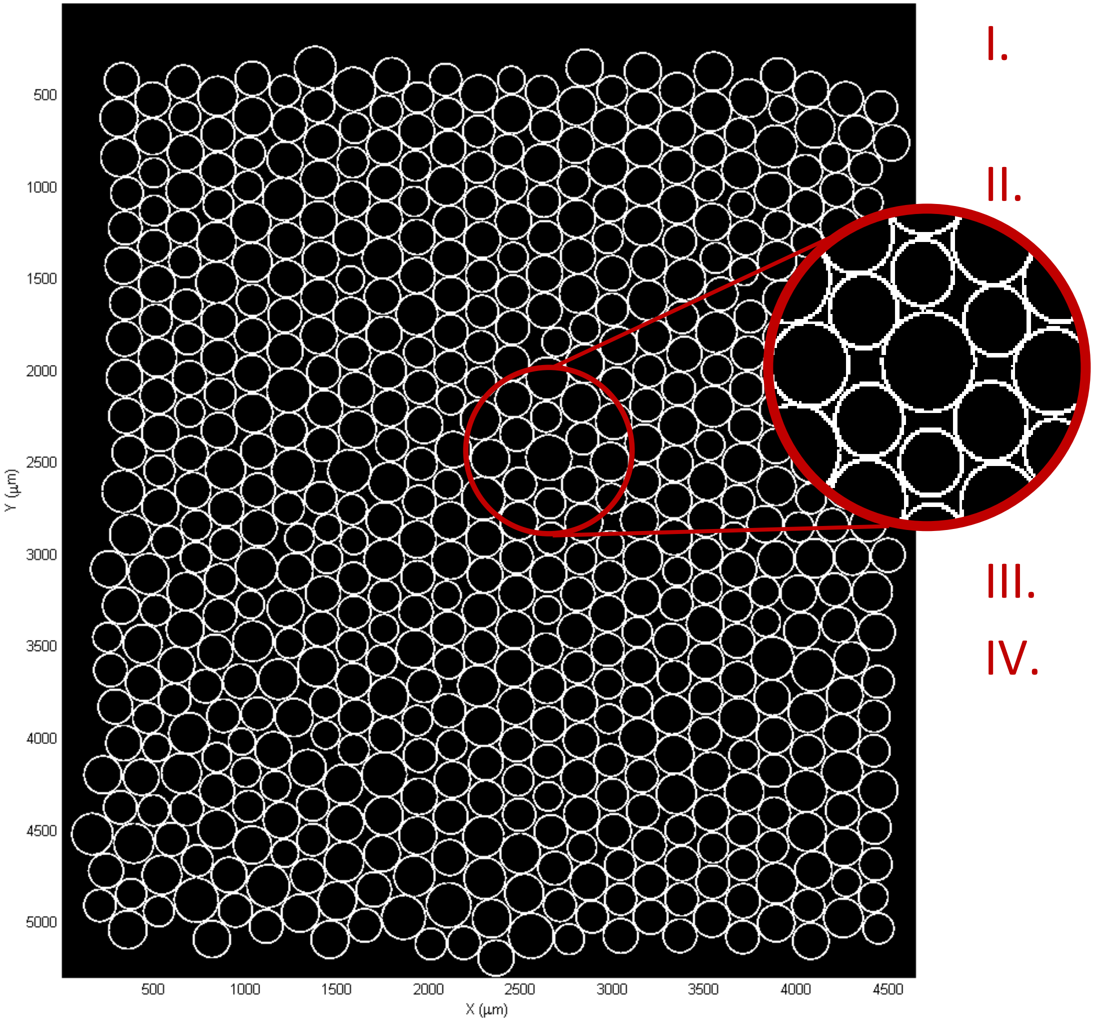
- generating ideal hexagonal crystal lattice (some particles may intersect)



Dispersion of particle radius (σ) on this picture is 10%.

Monte Carlo method

- reassembling particles using Monte Carlo (MC) method



I. Choosing random particle and random movement.

II. Counting system energy before and after shift, using Lennard-Jones potential.

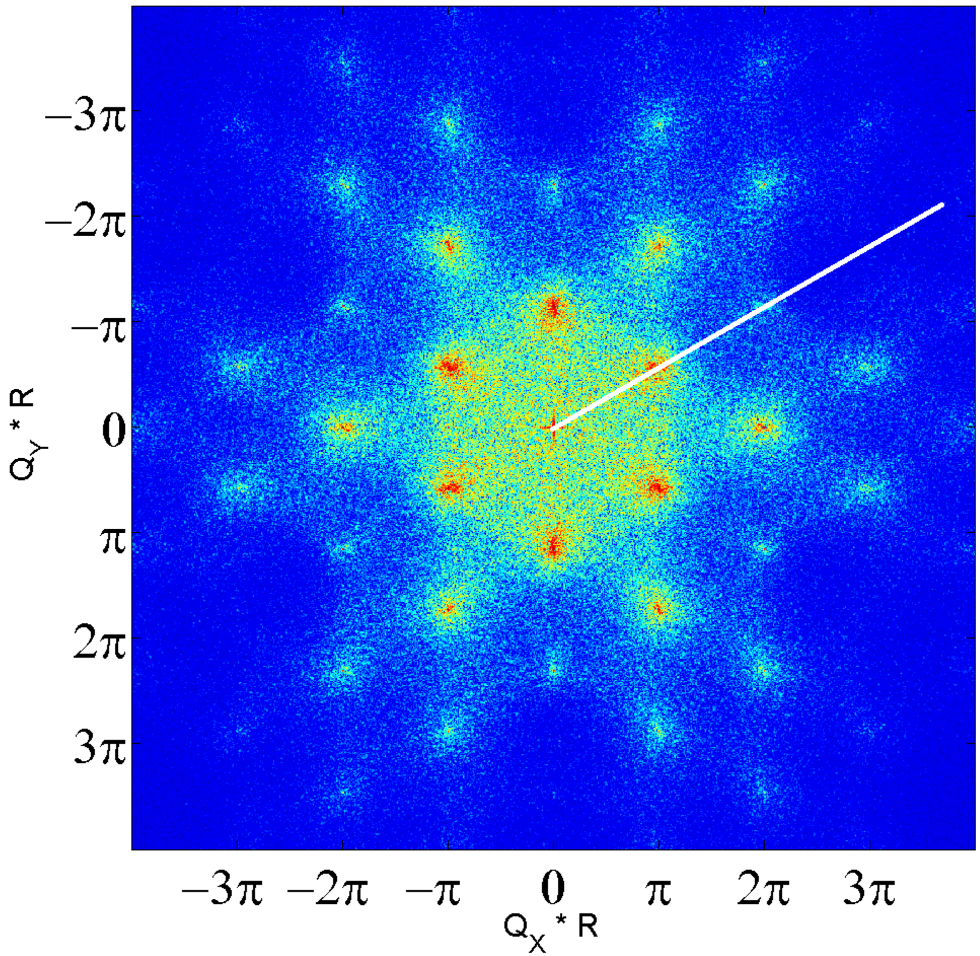
$$\boxed{U_{L-J} = \varepsilon\left[\left(\frac{r_0}{r}\right)^{12} + 2\left(\frac{r_0}{r}\right)^{6}\right]}$$

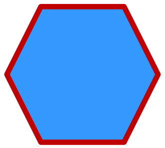
III. Calculating difference in energy.

IV. Accepting or declining the movement assuming Boltzmann statistics.

Calculation of X-ray diffraction

- generating diffraction pattern using two-dimensional Fourier transform (with flat Ewald sphere approximation)

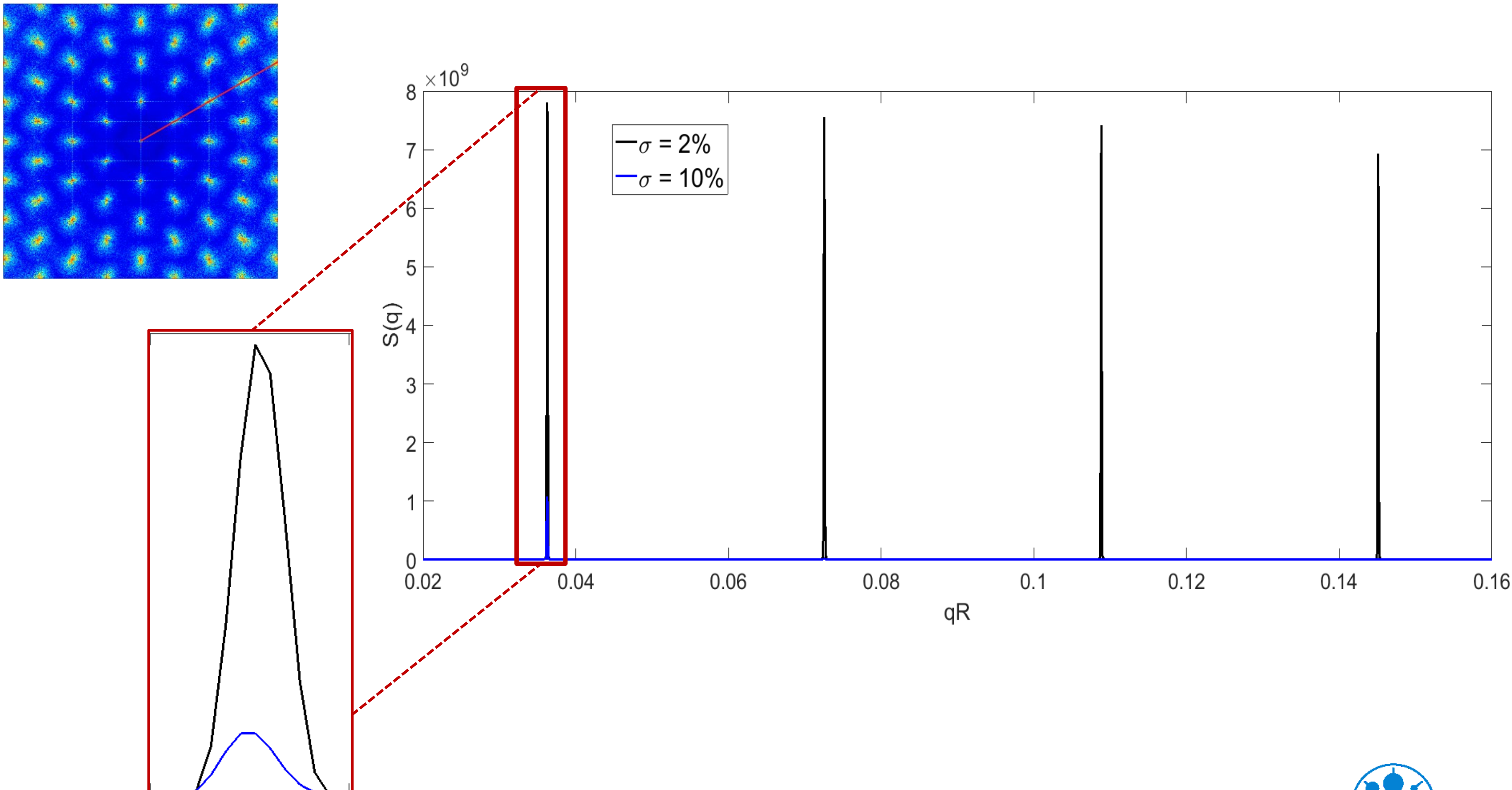




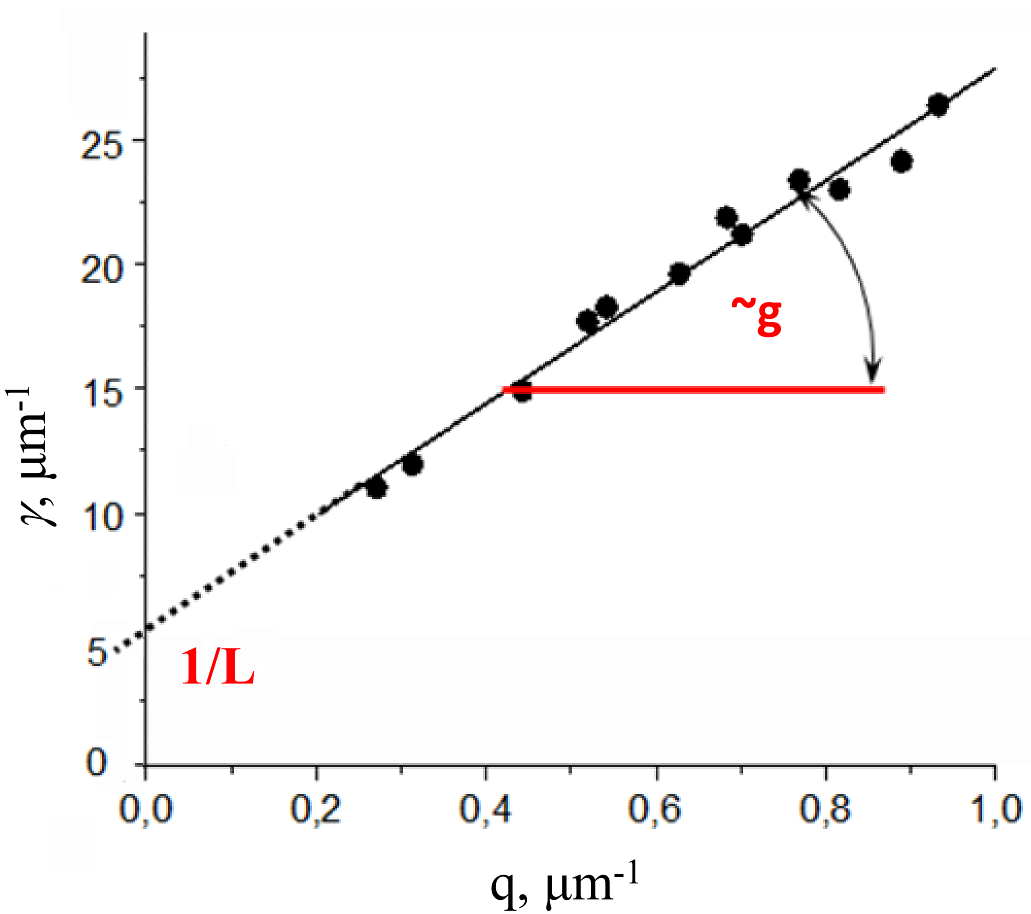
You may notice: Bragg peaks also have hexagonal structure!

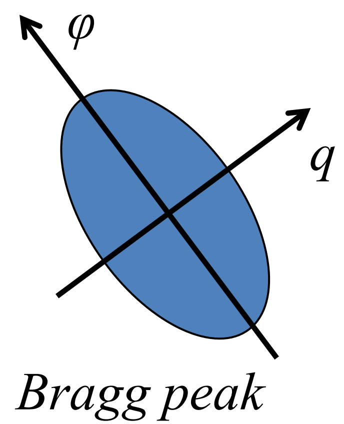
Radial cross section

- calculation of radial cross section of the structure factor for different dispersions (σ)



Williamson-Hall method





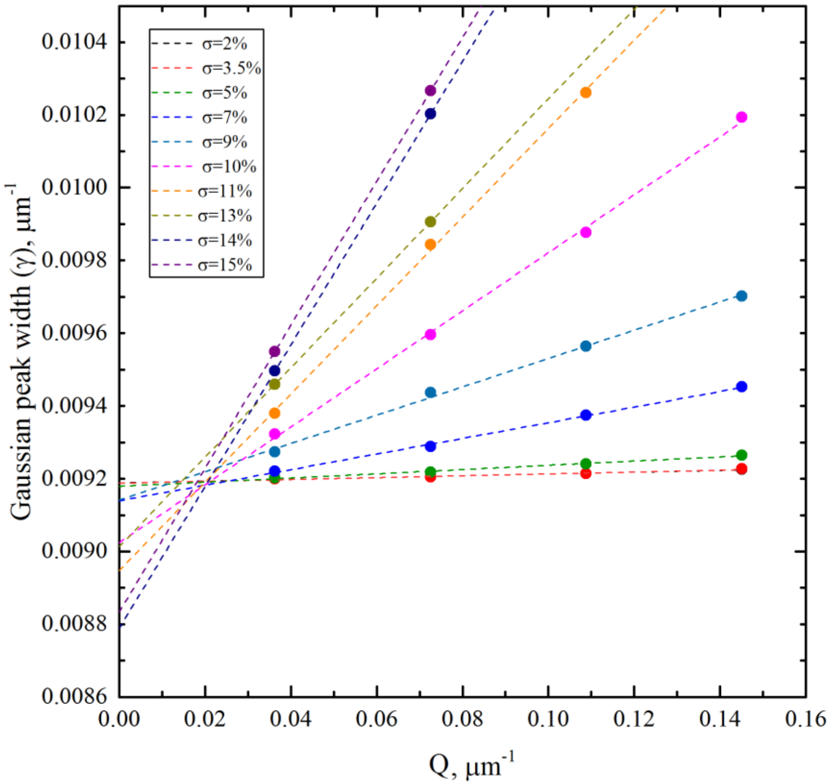
$$\boxed{\gamma(q) = \left(\frac{2\pi}{L}\right) + \left(g \cdot q\right)}$$

Coherent scattering domain size

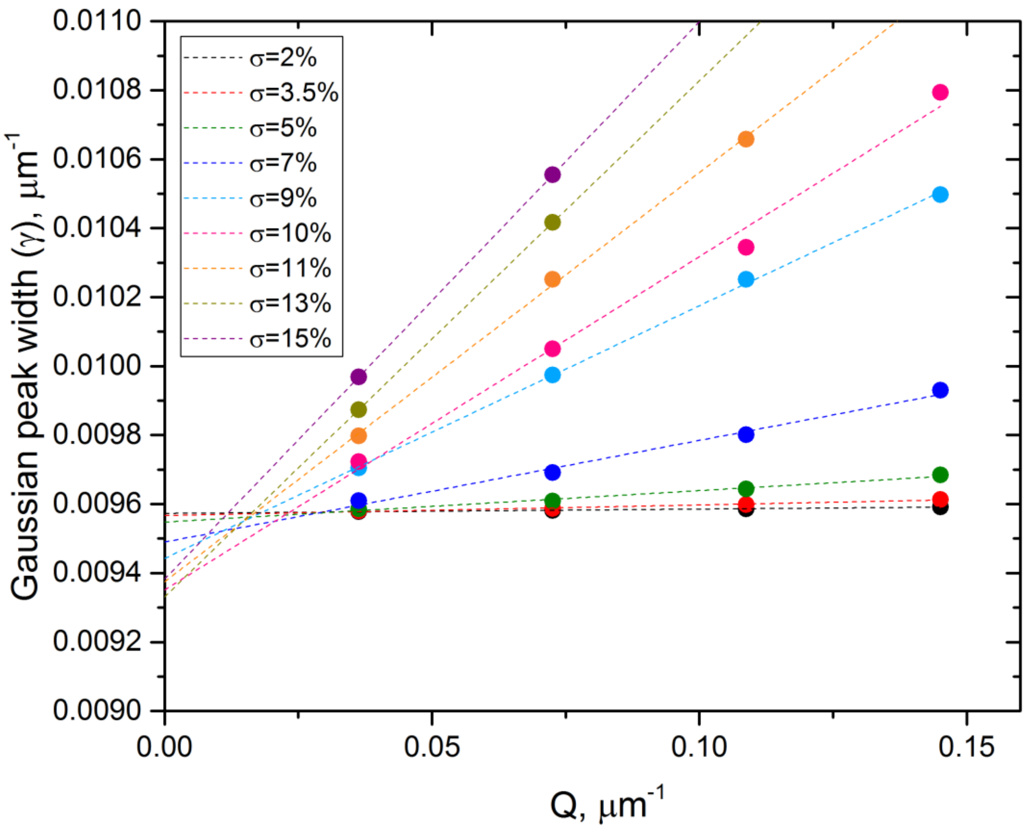
Strain

Williamson-Hall plot

❖ radial direction



❖ azimuthal direction

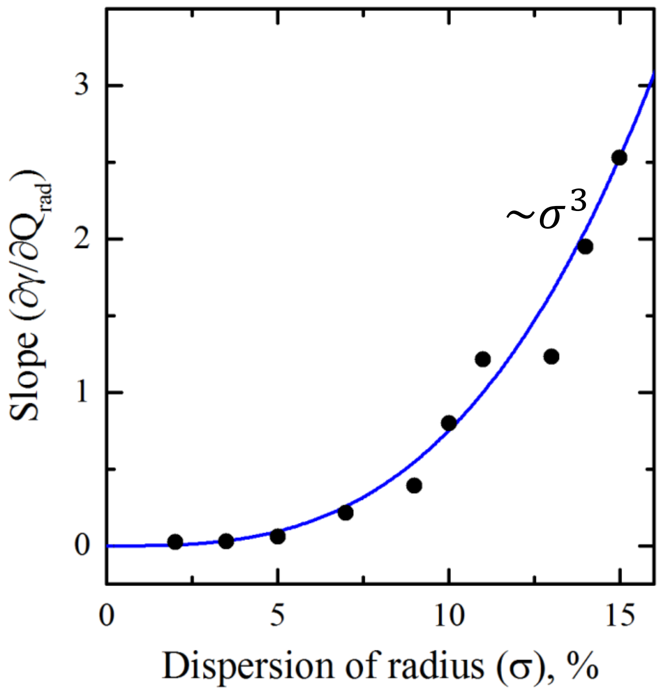


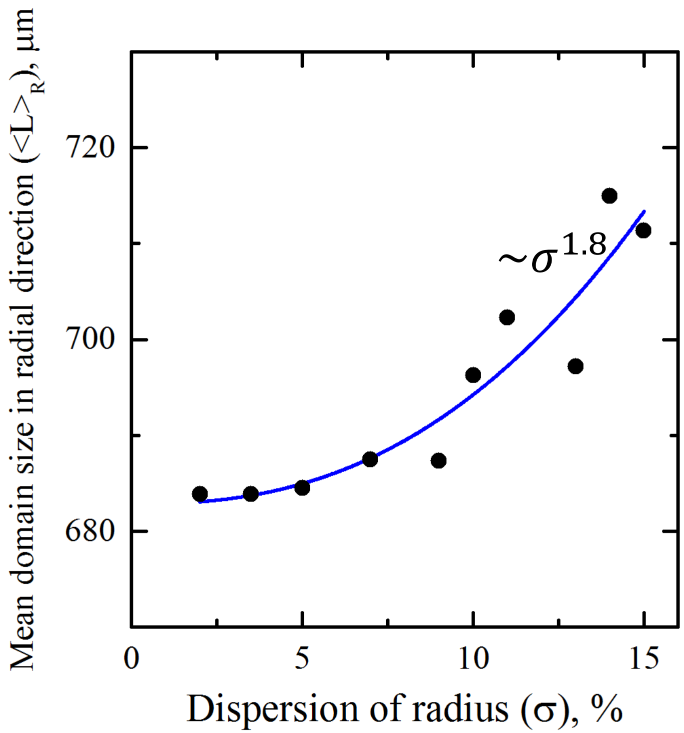
Slope and intersections in radial case

- calculating slope and intersections in radial direction

$$\gamma = \frac{2\pi}{\langle L\rangle_R} + \frac{\Delta d}{\langle d\rangle} \times q_{rad}$$

$\langle L\rangle_R$ - mean size of colloidal crystal domain in radial direction



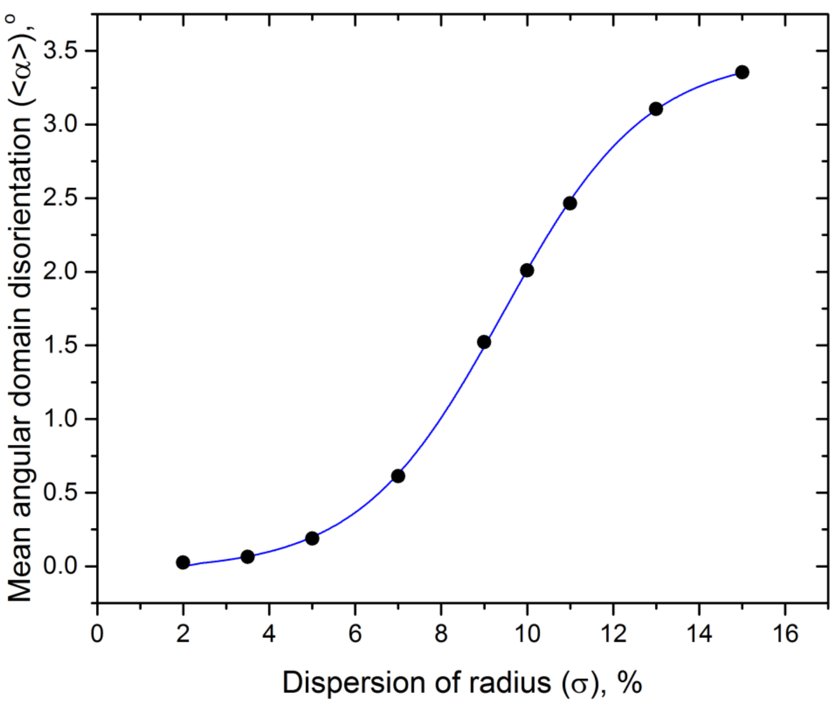


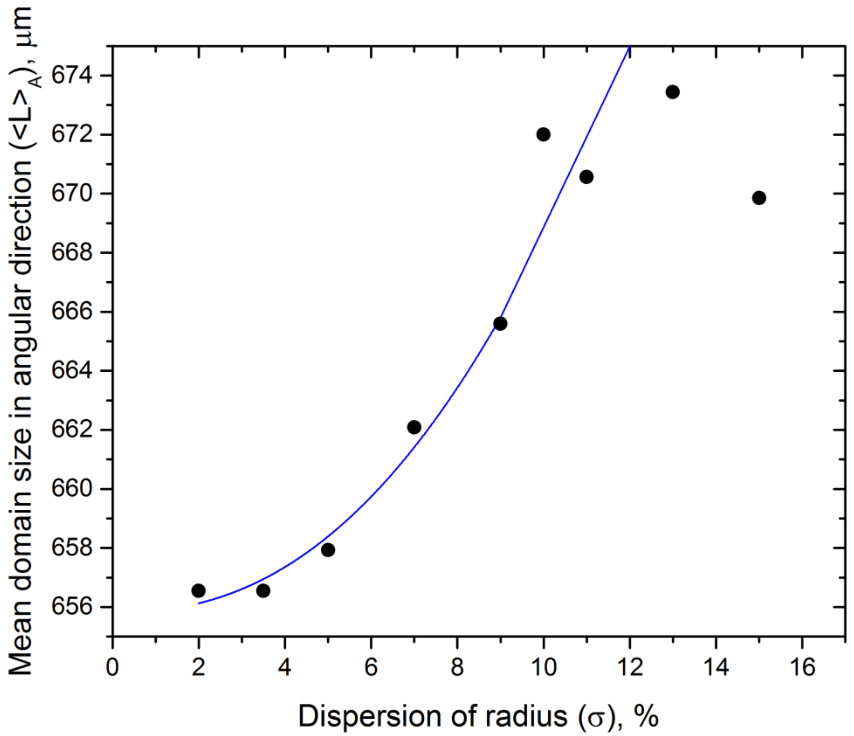
Slope and intersections in azimuthal case

- calculating slope and intersections in azimuthal direction

$$\gamma = \frac{2\pi}{\langle L \rangle_A} + \tan\alpha \times q_{rad}$$

$\langle L \rangle_A$ - mean size of colloidal crystal domain in azimuthal direction





Summary and conclusions

What have we done?

- colloidal crystal lattice generation algorithm
- X-ray diffraction calculation algorithm
- application Williamson-Hall approach for our model

What have we obtained?

- colloid particles domain size behavior in dependence on dispersion of particle radius (σ)
- increasement of fluctuation of interparticle distances in dependence on dispersion of particle radius (σ)
- angular domain disorientation dependence on dispersion of particle radius (σ)

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Three-dimensional case

- we managed to get all the scripts working but it takes a lot of time to get results we need, because algorithm can't be parallelised