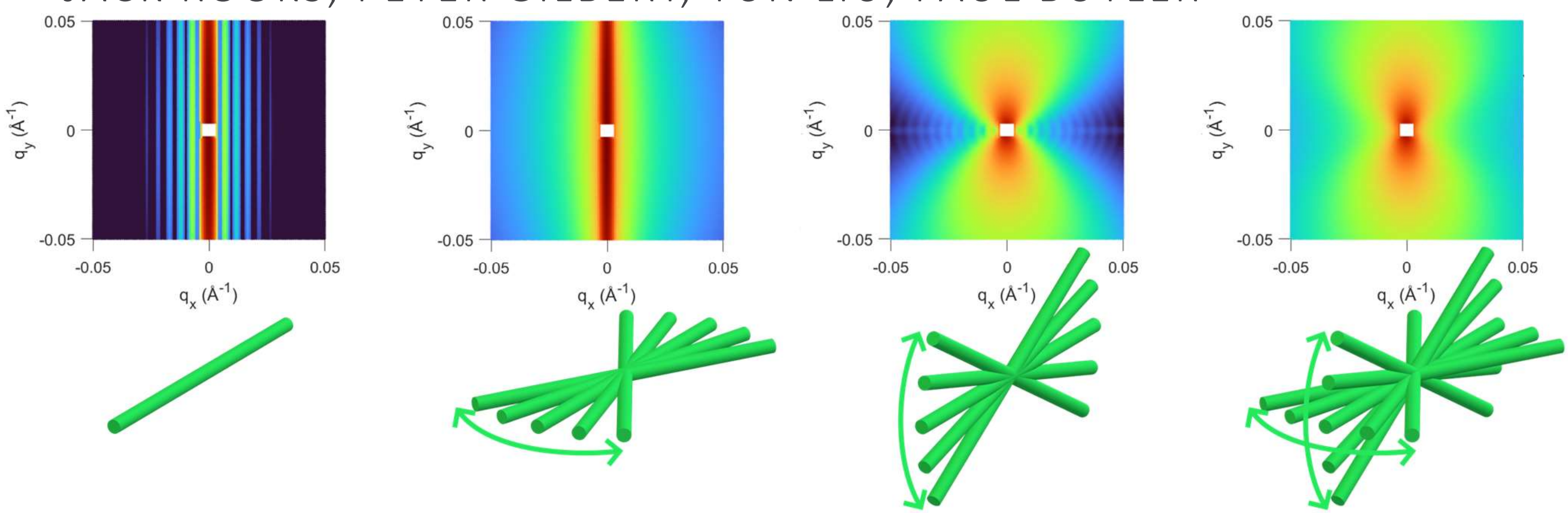
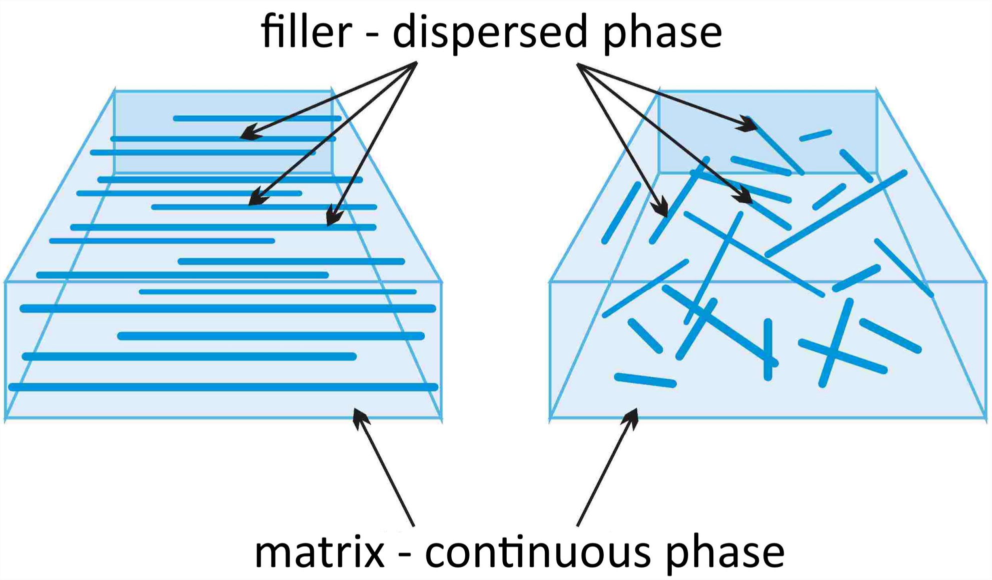
Particle orientation in soft materials from small-angle neutron scattering

JACK ROOKS, PETER GILBERT, YUN LIU, PAUL BUTLER



Orientation affects material properties

Material properties depend on orientation/alignment



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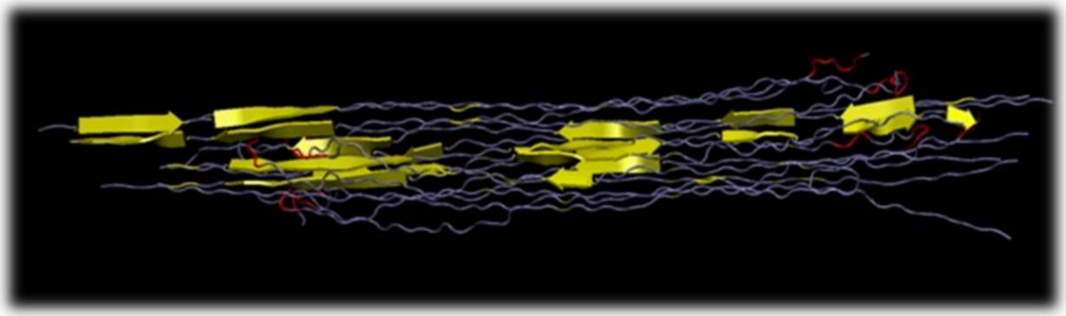
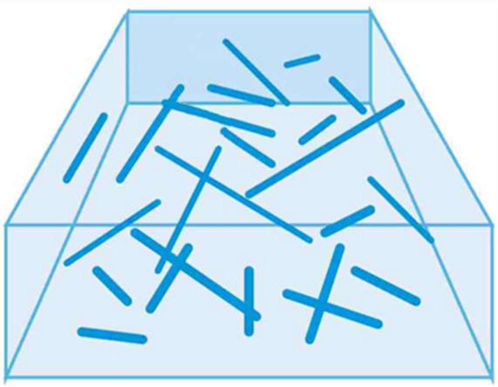
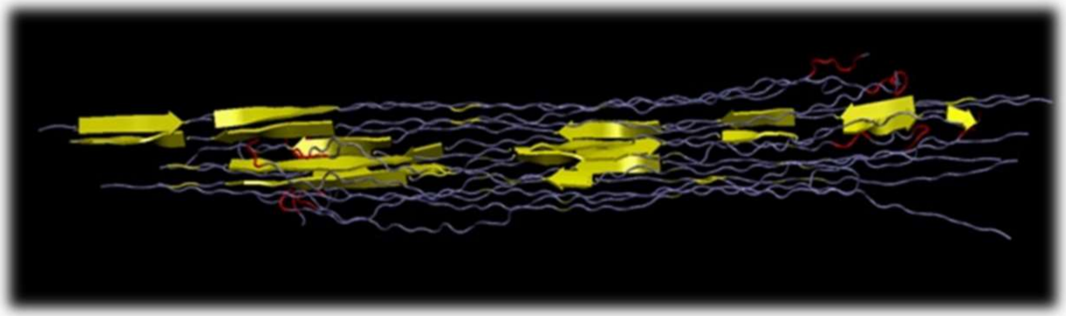


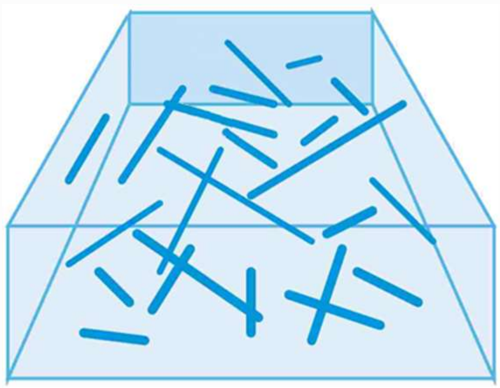
Spider silk molecular structure



Orientation affects material properties

Material properties depend on orientation/alignment

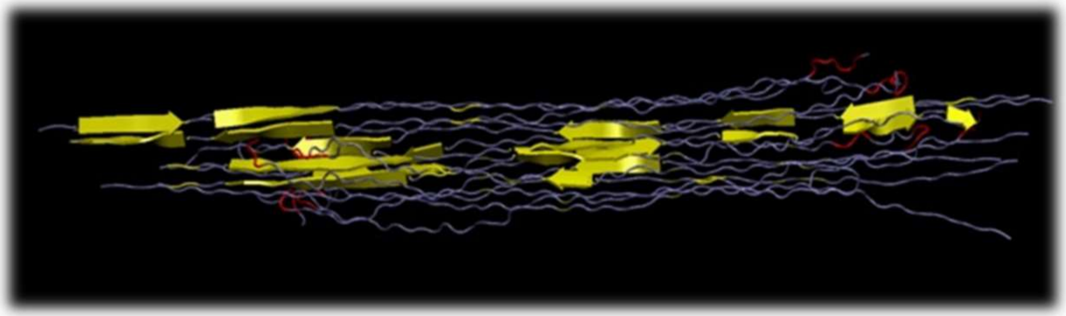


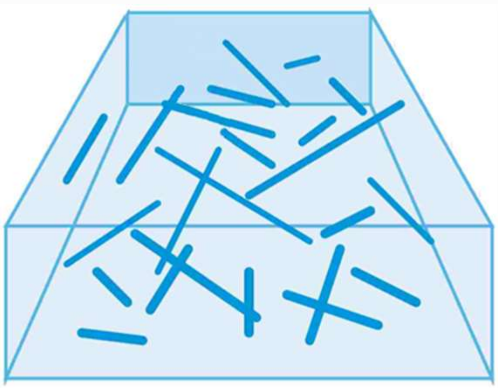


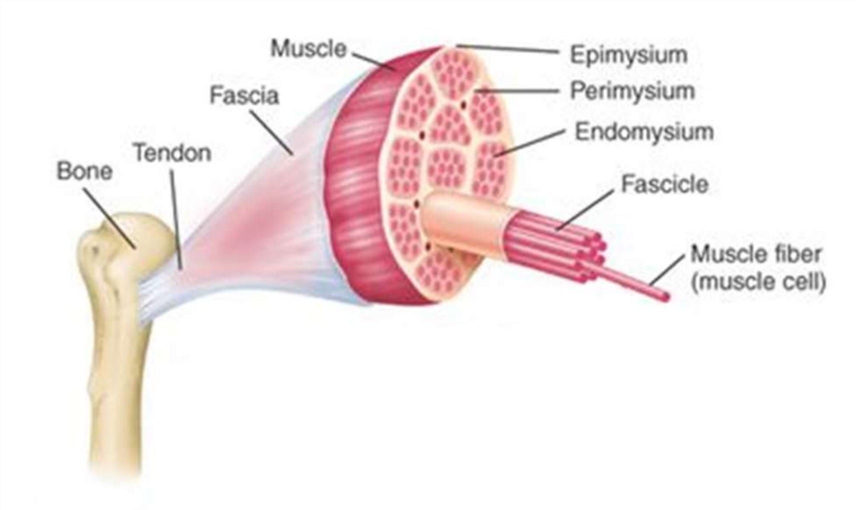
Rebar in concrete

Orientation affects material properties

Material properties depend on orientation/alignment



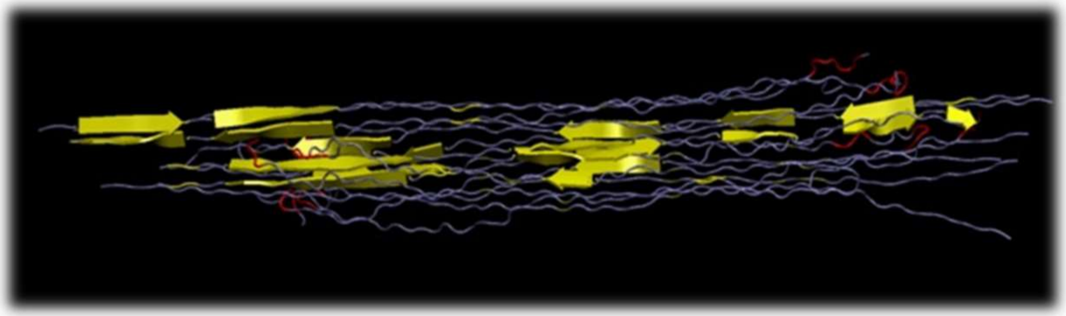


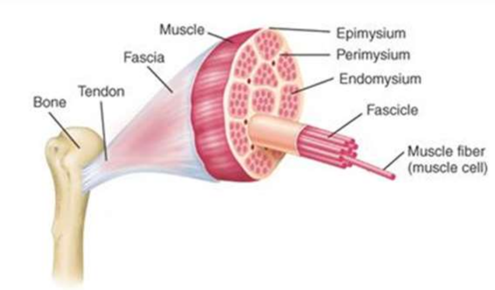


Muscle cells

Orientation affects material properties

Material properties depend on orientation/alignment

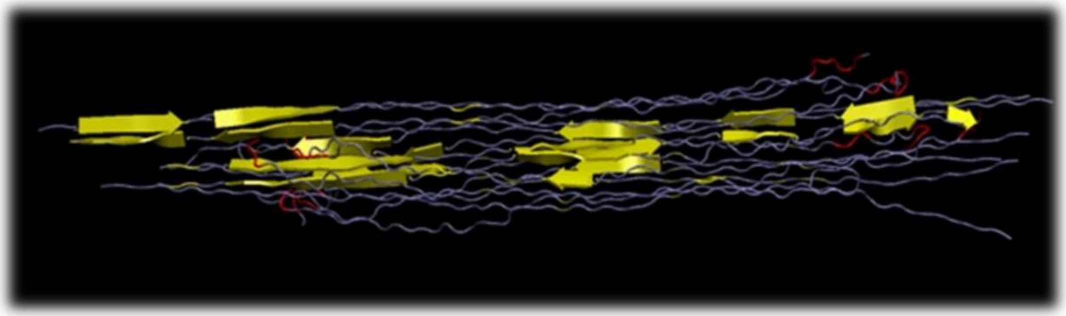


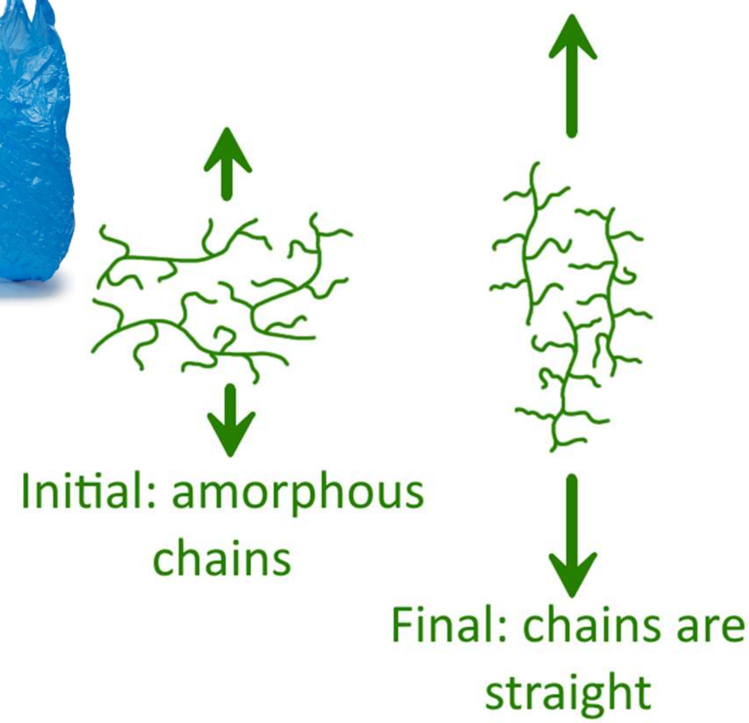


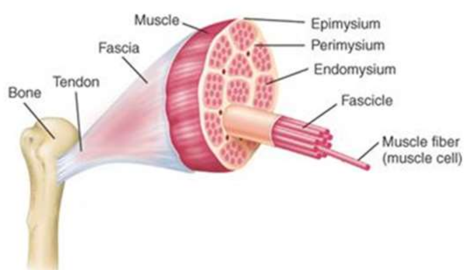
Plastic bags

Orientation affects material properties

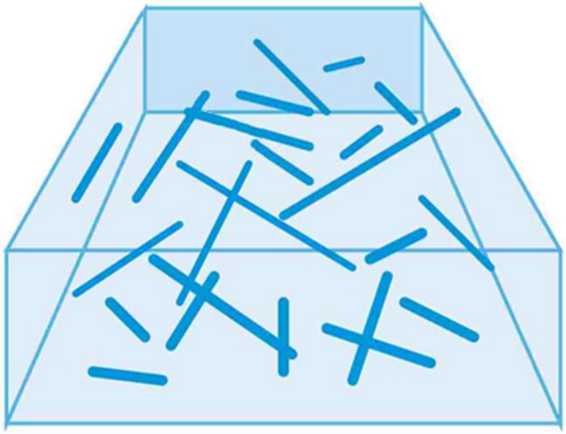
Material properties depend on orientation/alignment







Neutron scattering to measure particles



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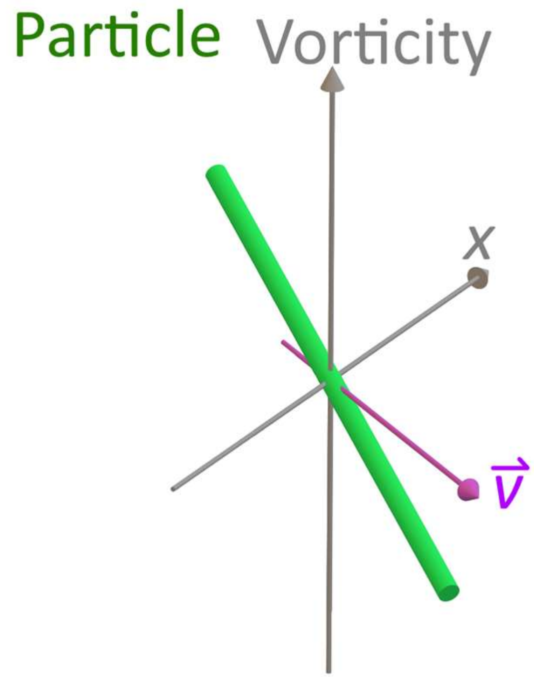

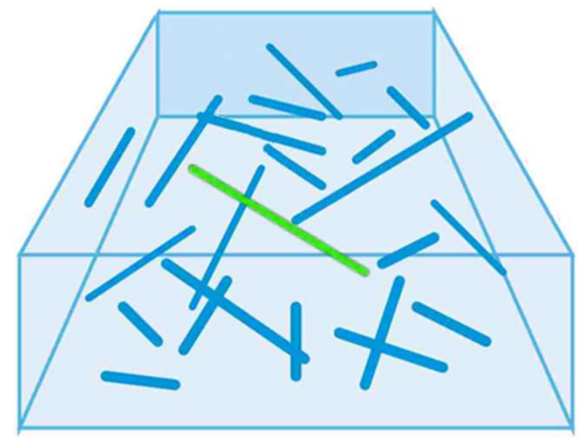

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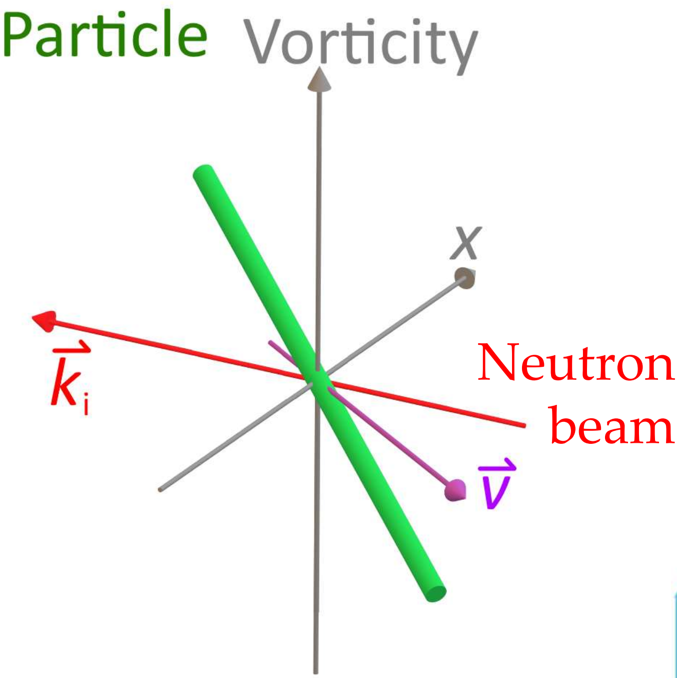

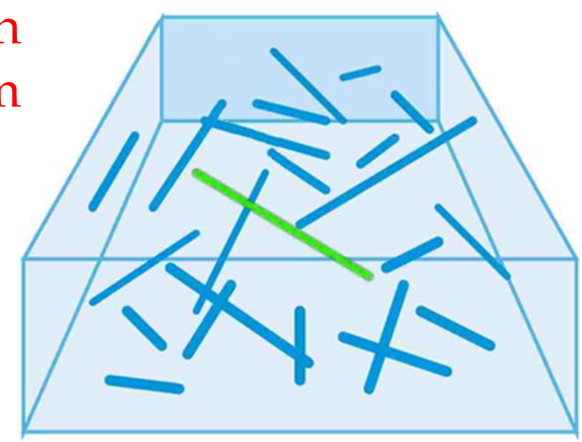

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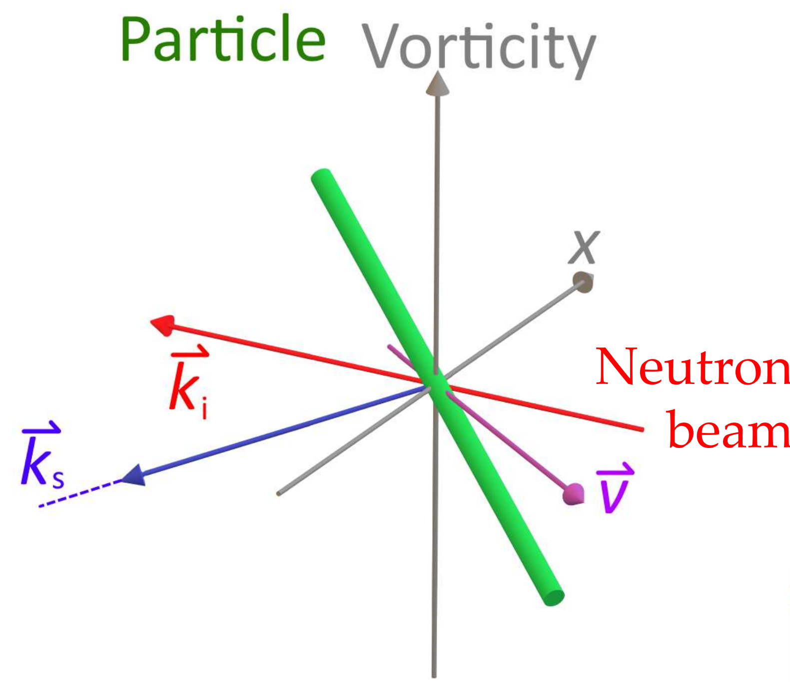
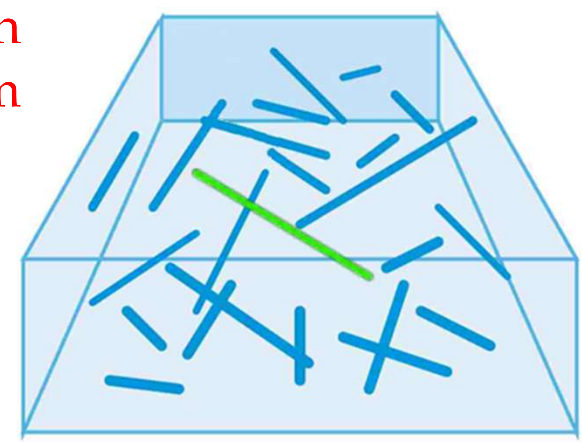
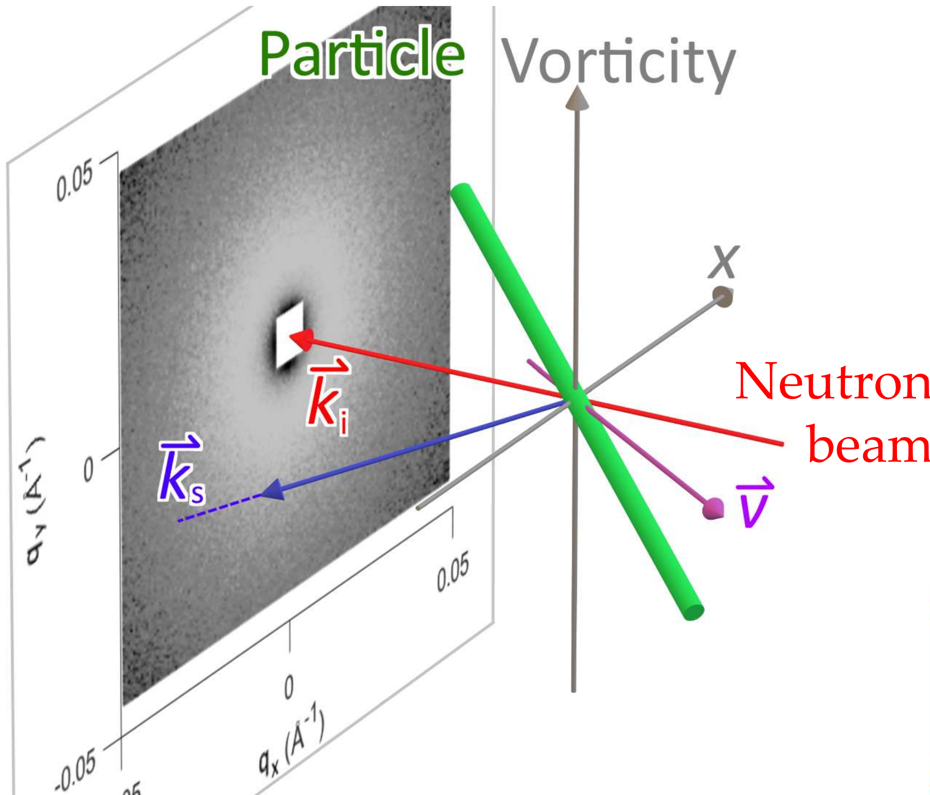
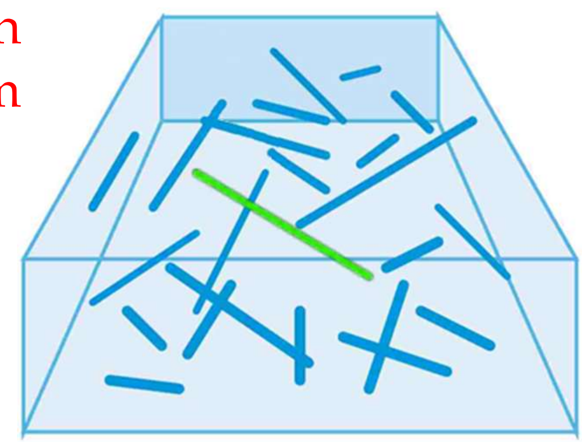


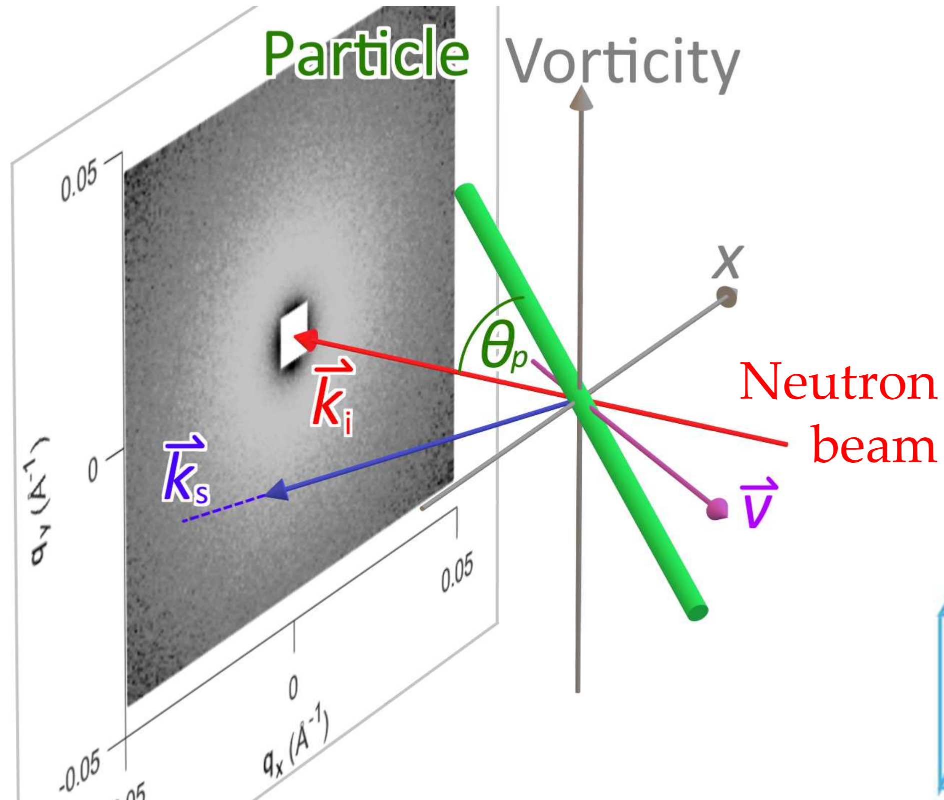


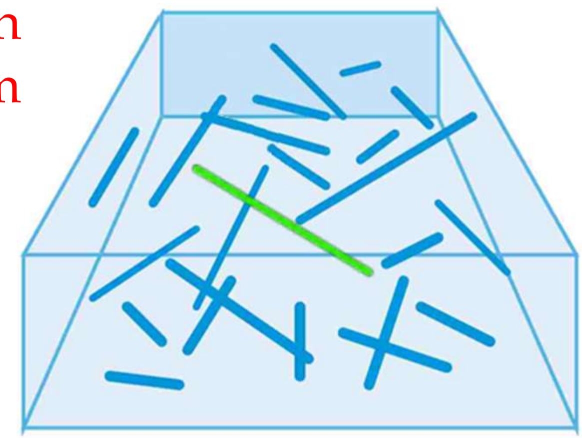
Neutron scattering to measure particles



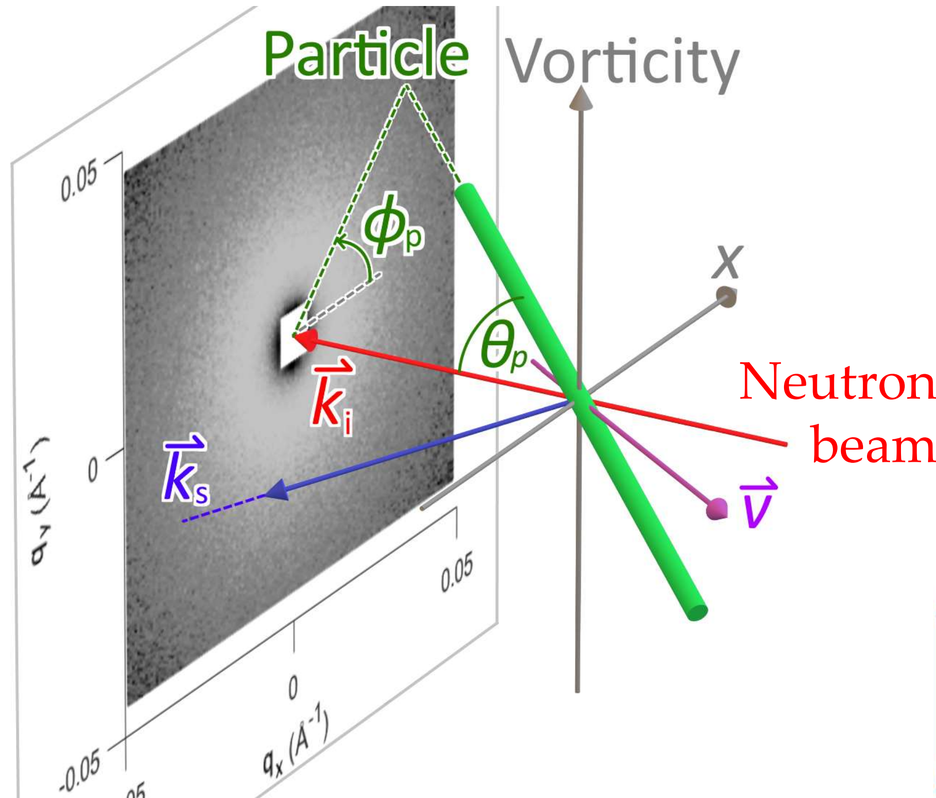


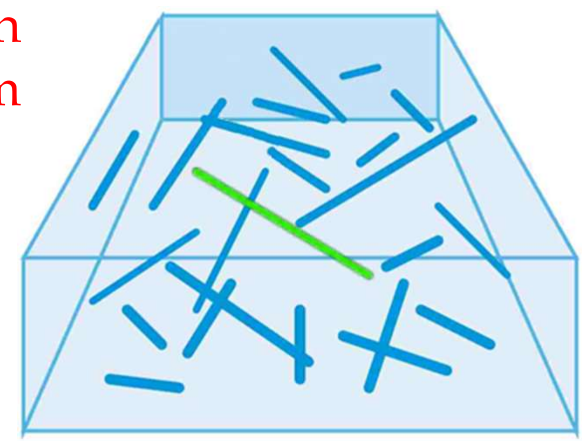
Neutron scattering to measure particles



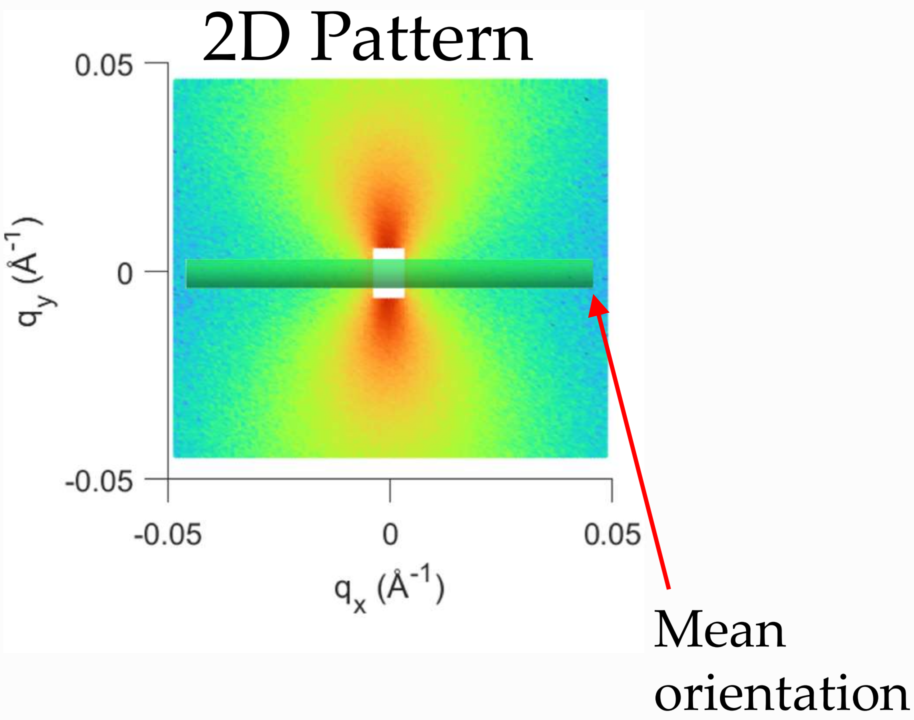


Neutron scattering to measure particles



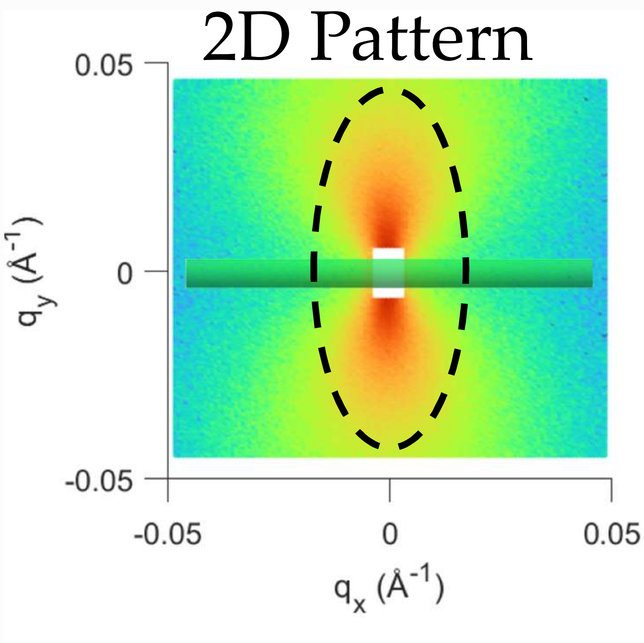


What neutron scattering tells us



Small angle neutron scattering (SANS)

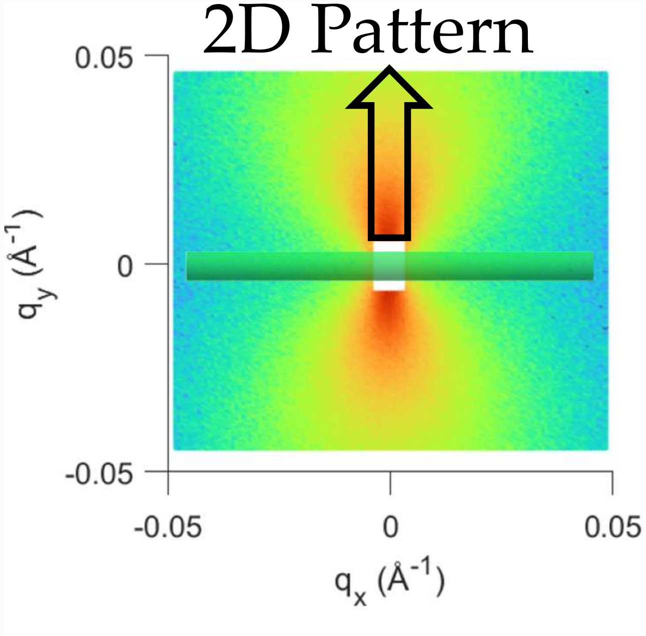
What neutron scattering tells us



Small angle neutron scattering (SANS)

- Peak: mean orientation

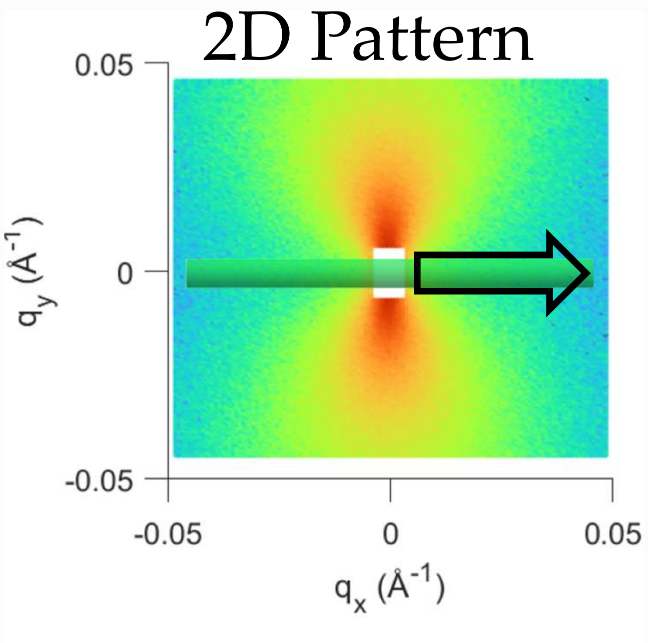
What neutron scattering tells us



- Peak: mean orientation
- Perpendicular: radius

Small angle neutron scattering (SANS)

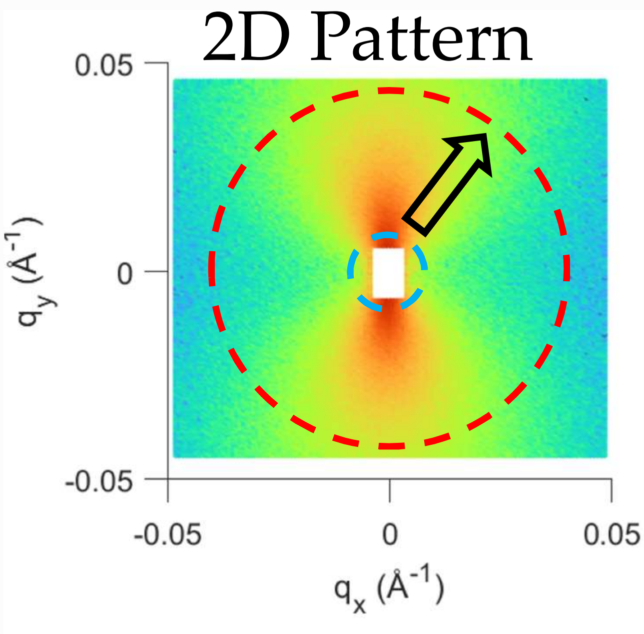
What neutron scattering tells us



Small angle neutron scattering (SANS)

- Peak: mean orientation
- Perpendicular: radius
- Parallel: length

What neutron scattering tells us

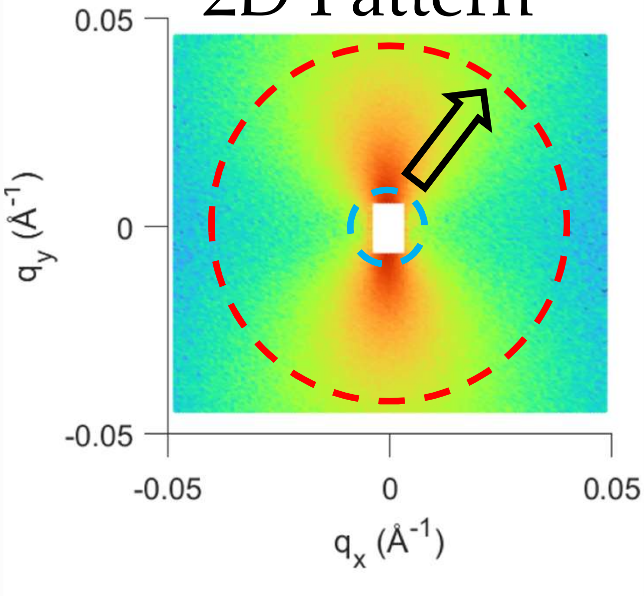


Small angle neutron scattering (SANS)

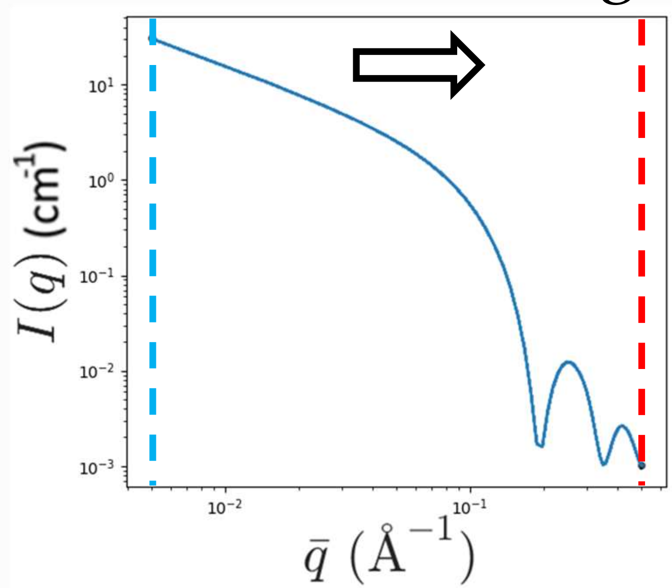
- Peak: mean orientation
- Perpendicular: radius
- Parallel: length

What neutron scattering tells us

2D Pattern

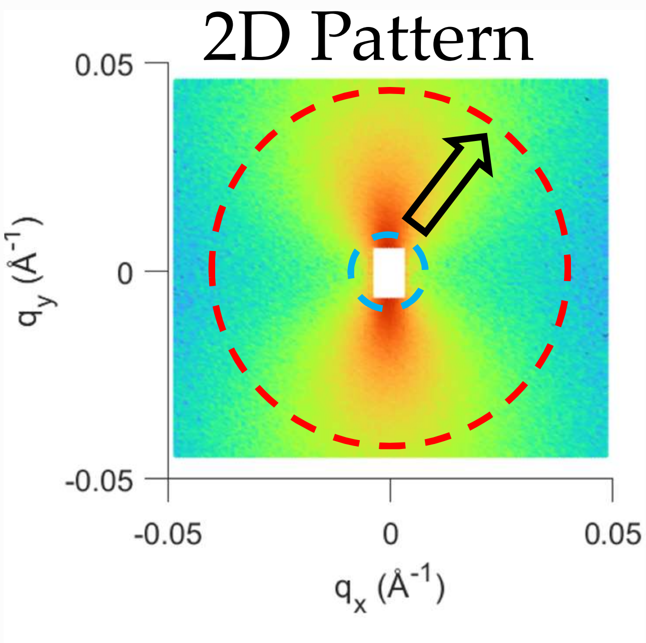


1D Circular Average

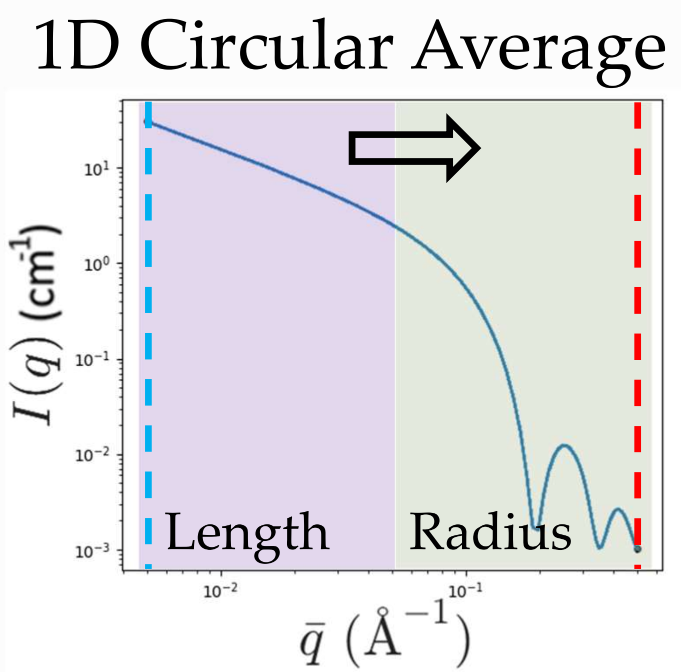


- Peak: mean orientation
- Perpendicular: radius
- Parallel: length

What neutron scattering tells us

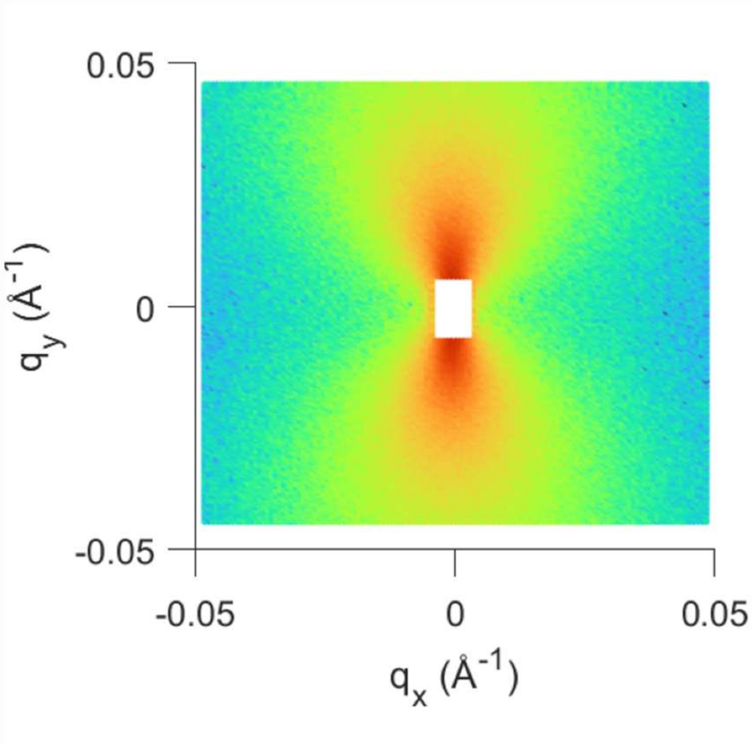


- Peak: mean orientation
- Perpendicular: radius
- Parallel: length



- Shape: particle morphology
- Position: particle dimensions

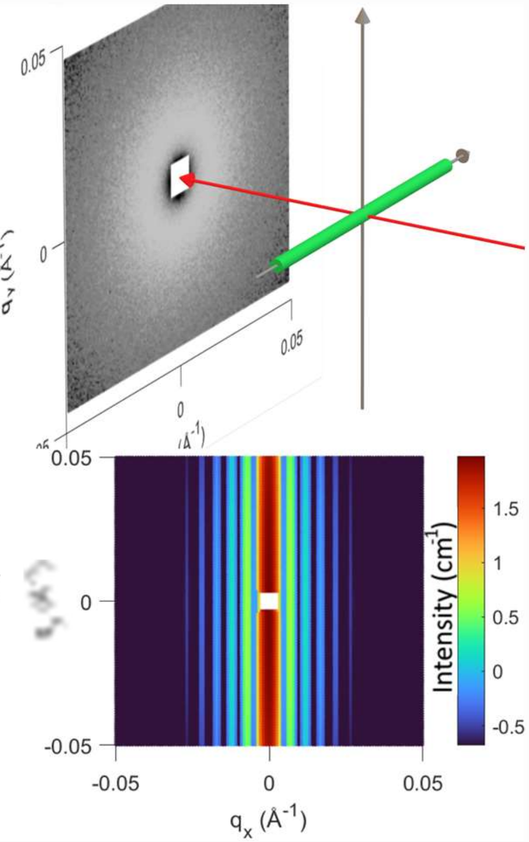
Orientation from neutron scattering



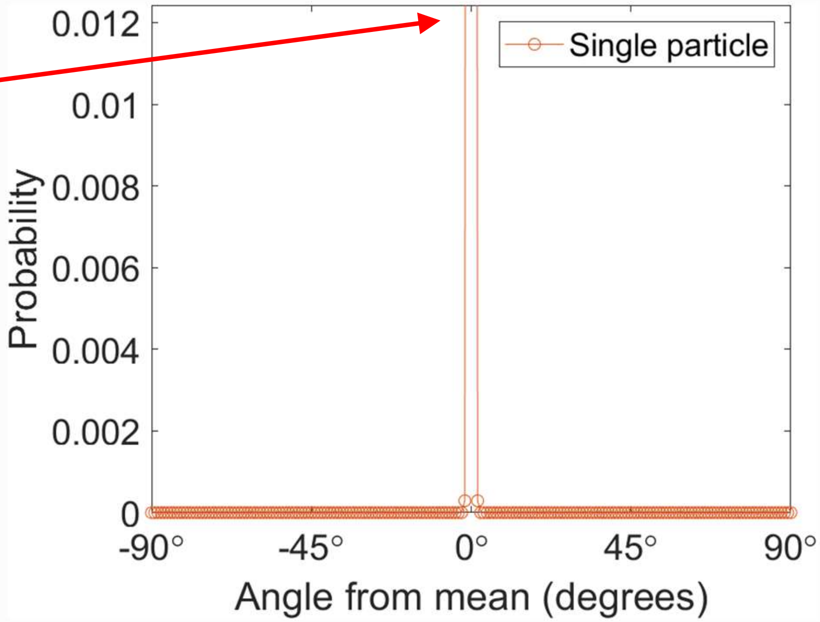
Question:

Can we obtain orientation information from SANS?

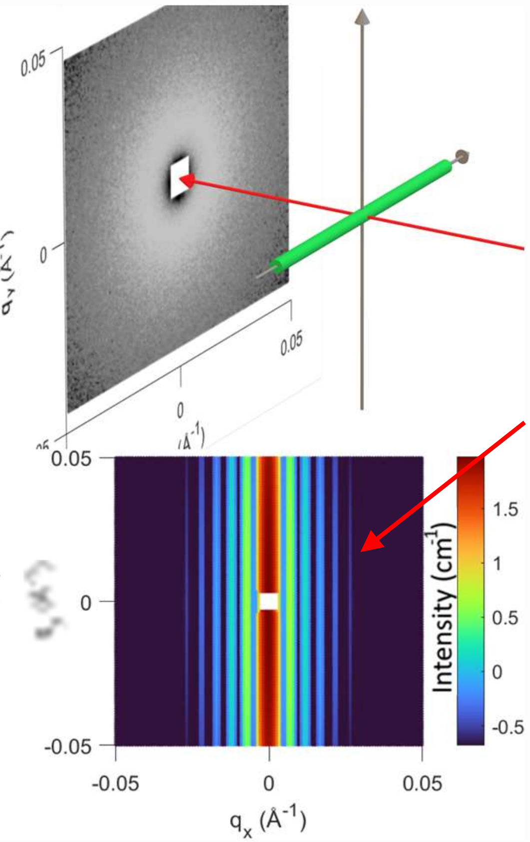
Orientation from neutron scattering



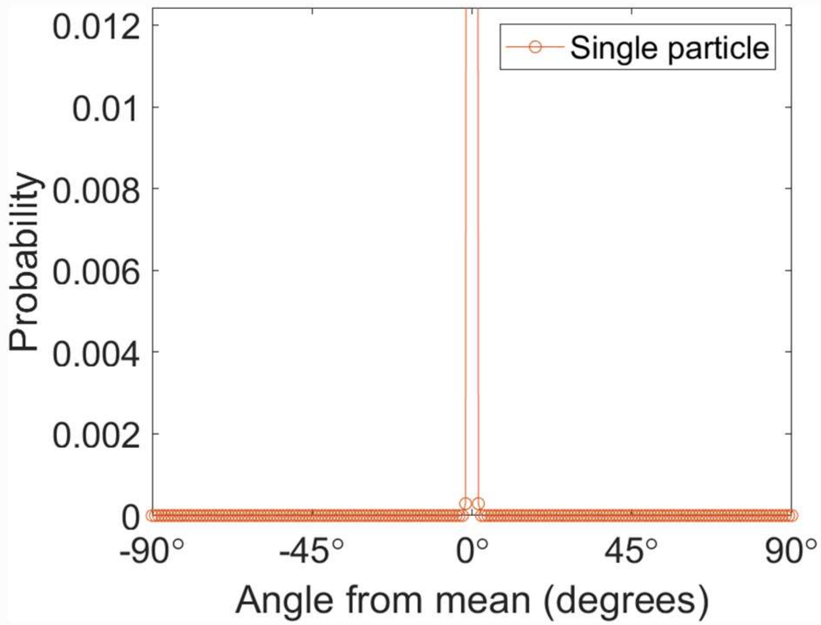
All particles have mean orientation



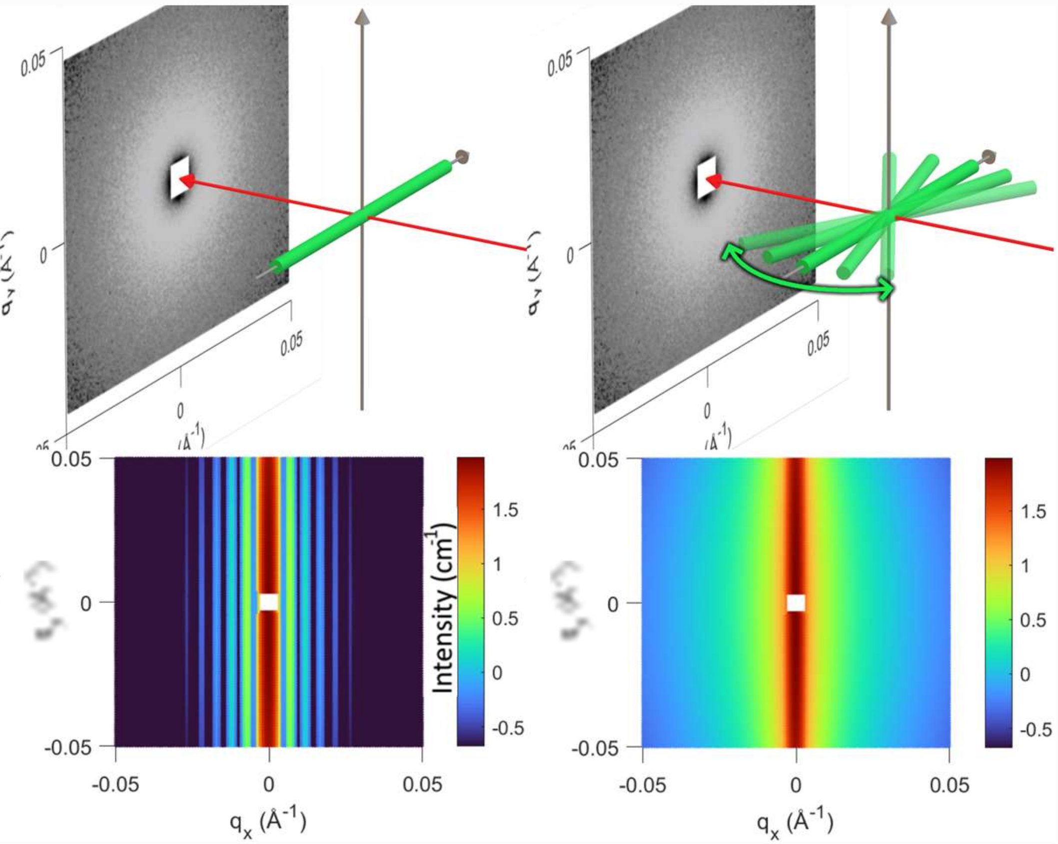
Orientation from neutron scattering



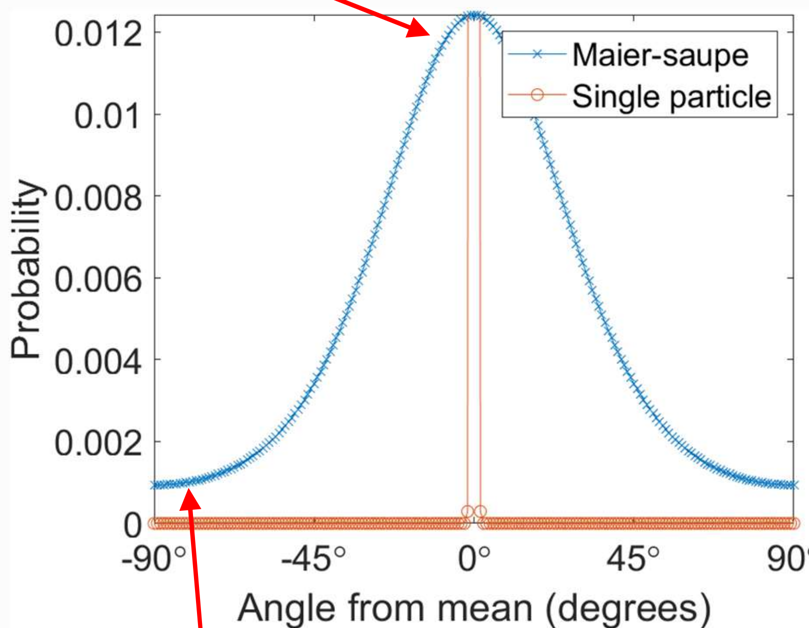
Sharp features, very straight



Orientation from neutron scattering

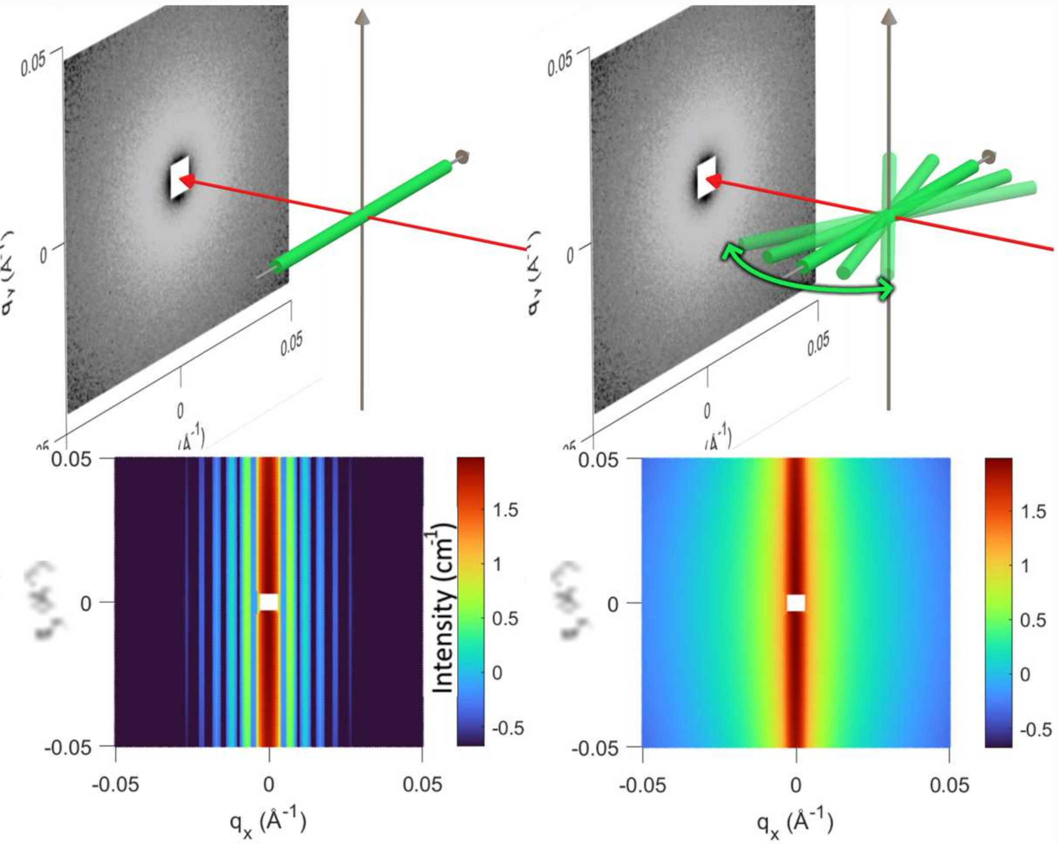


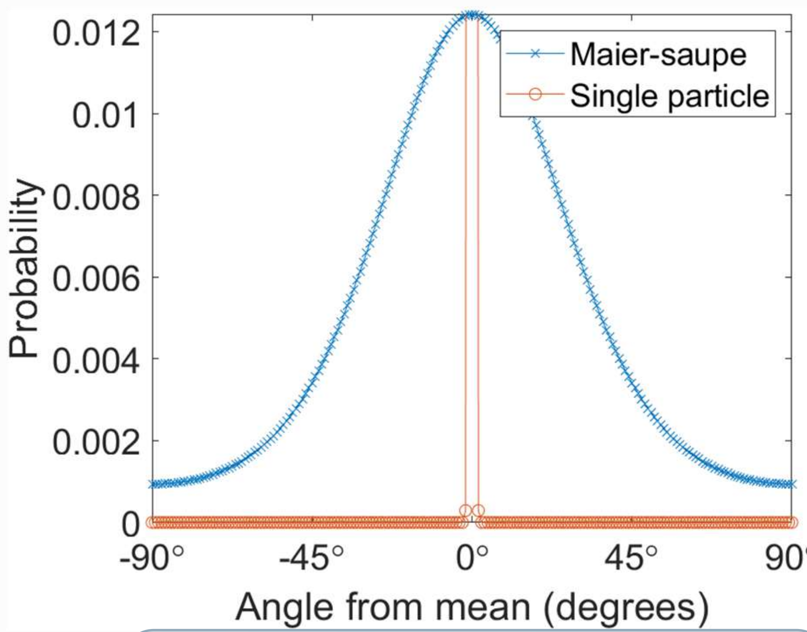
Most particles have mean orientation



Some particles point other directions

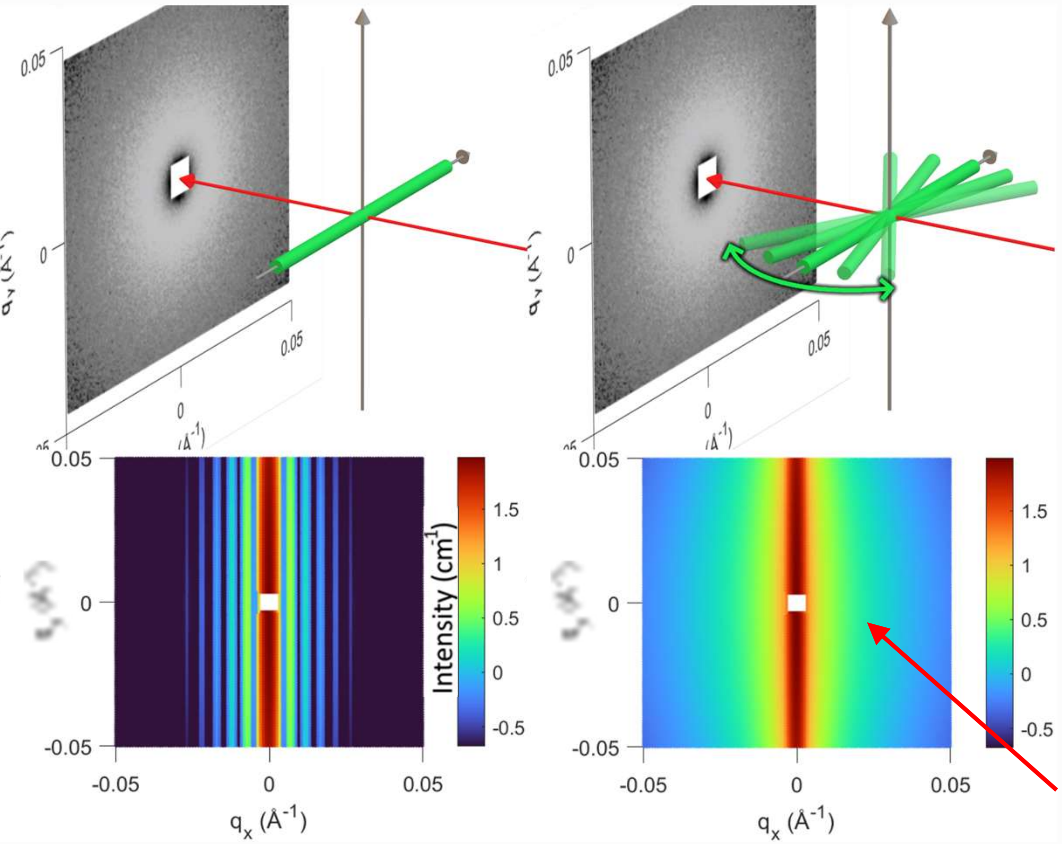
Orientation from neutron scattering

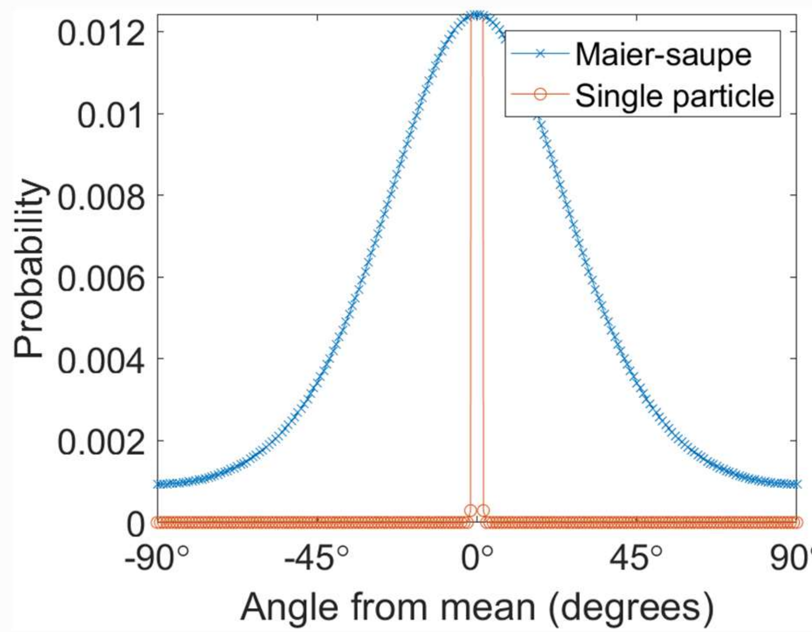




A width parameter describes distribution

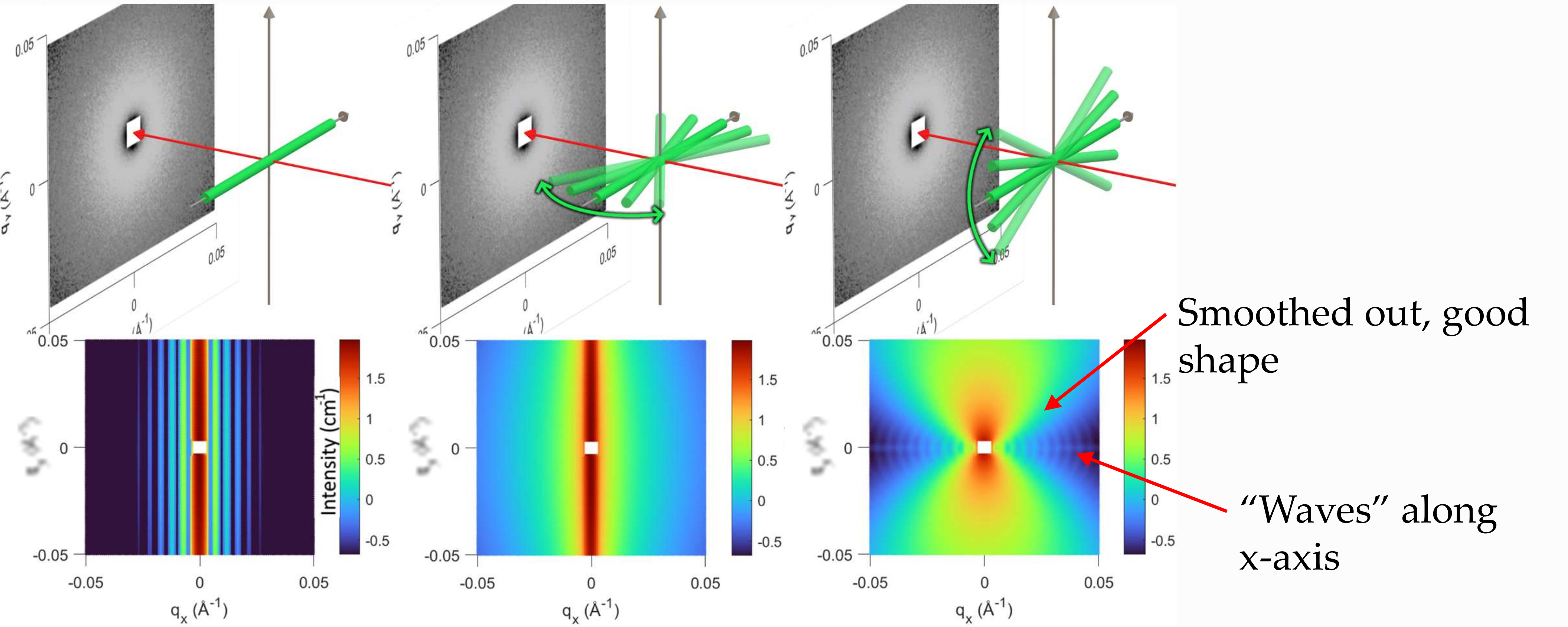
Orientation from neutron scattering



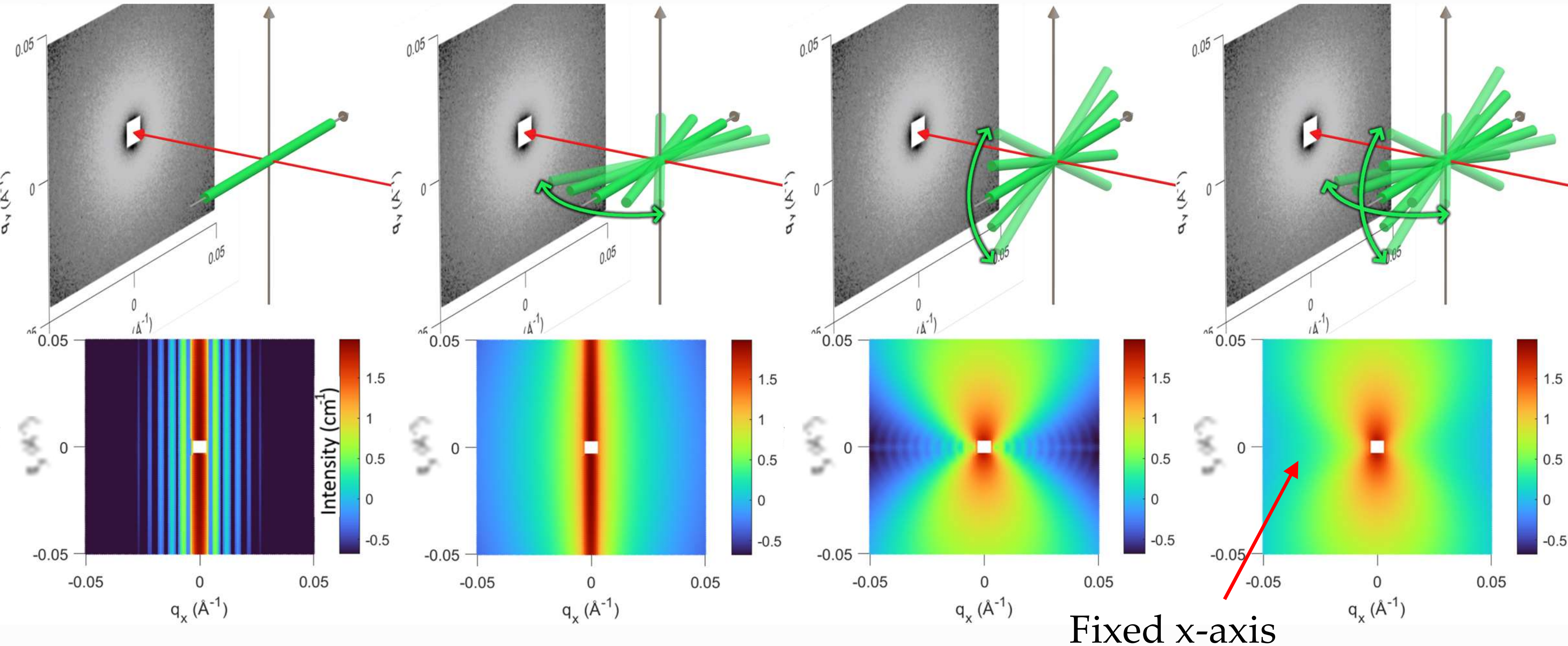


Smoothed out features. Still very straight

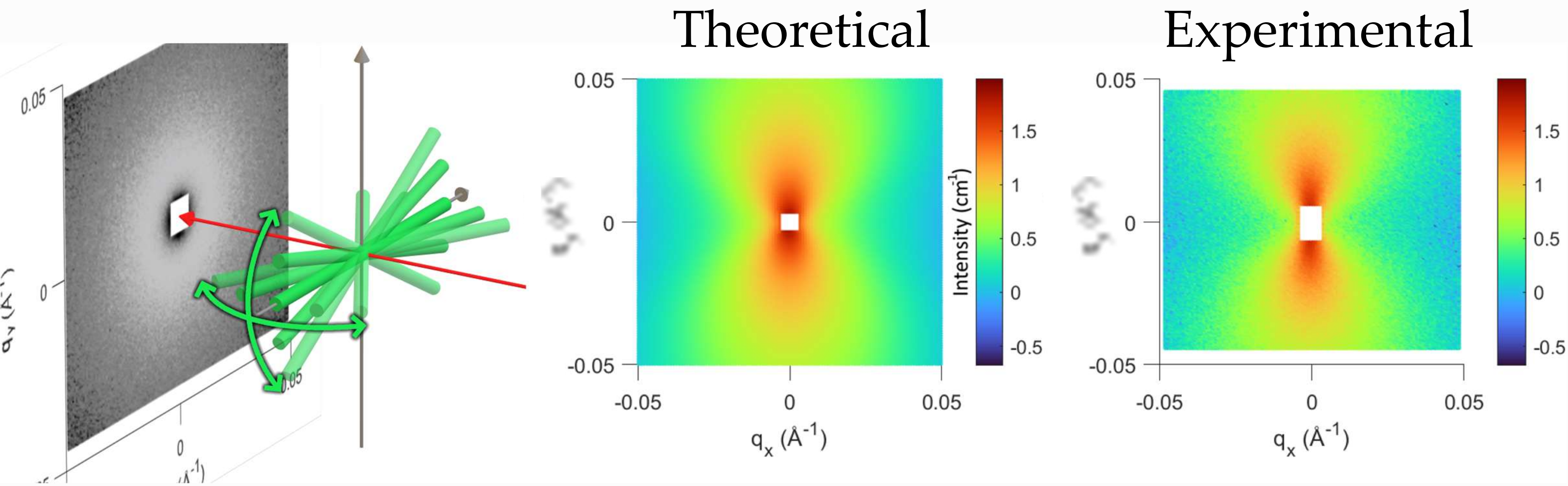
Orientation from neutron scattering



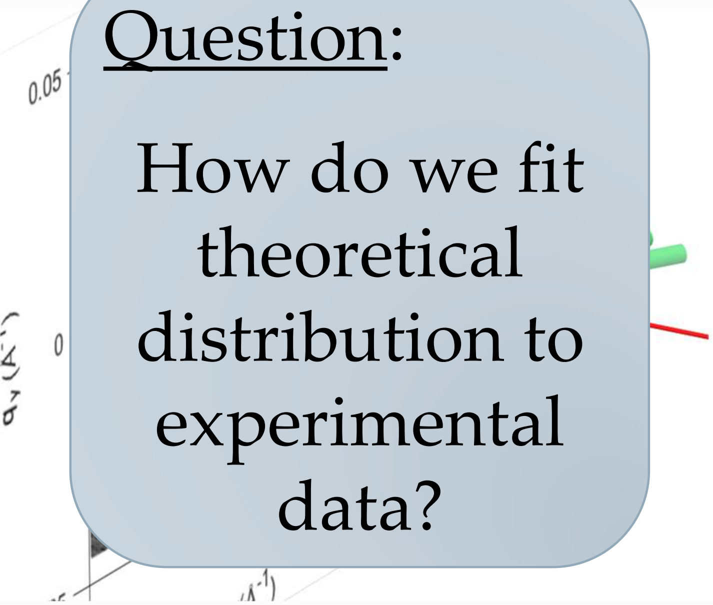
Orientation from neutron scattering



Orientation from neutron scattering

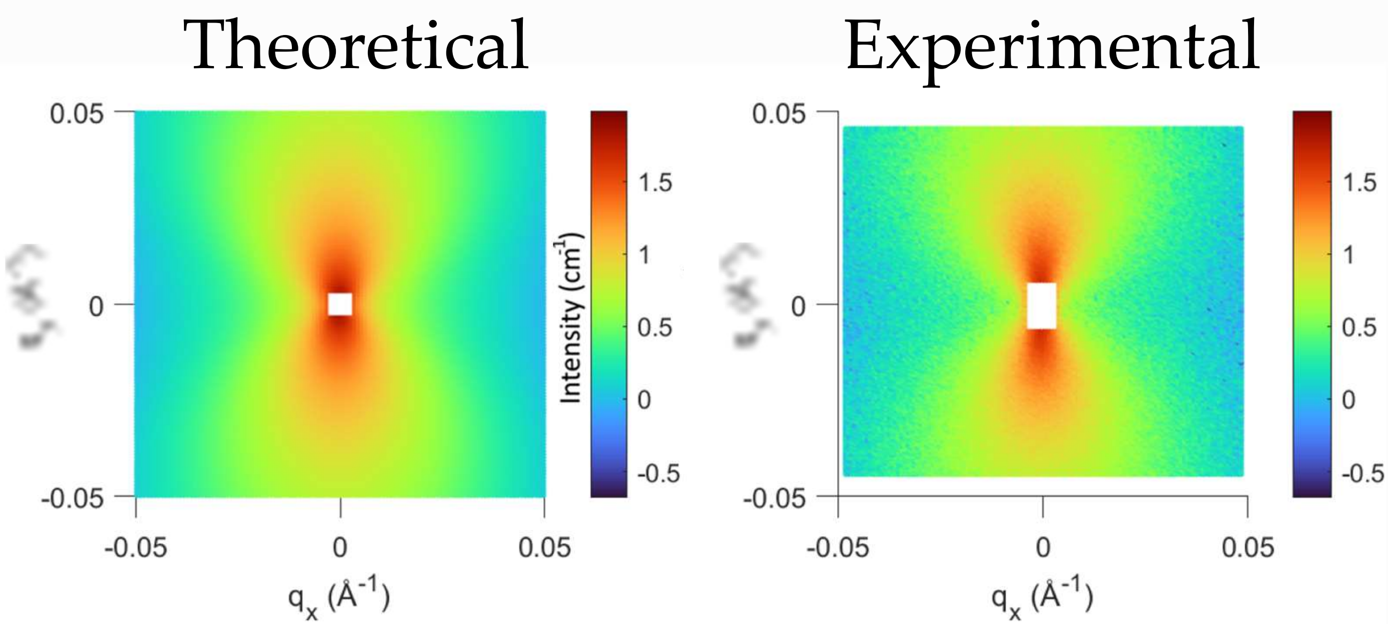


Orientation from neutron scattering

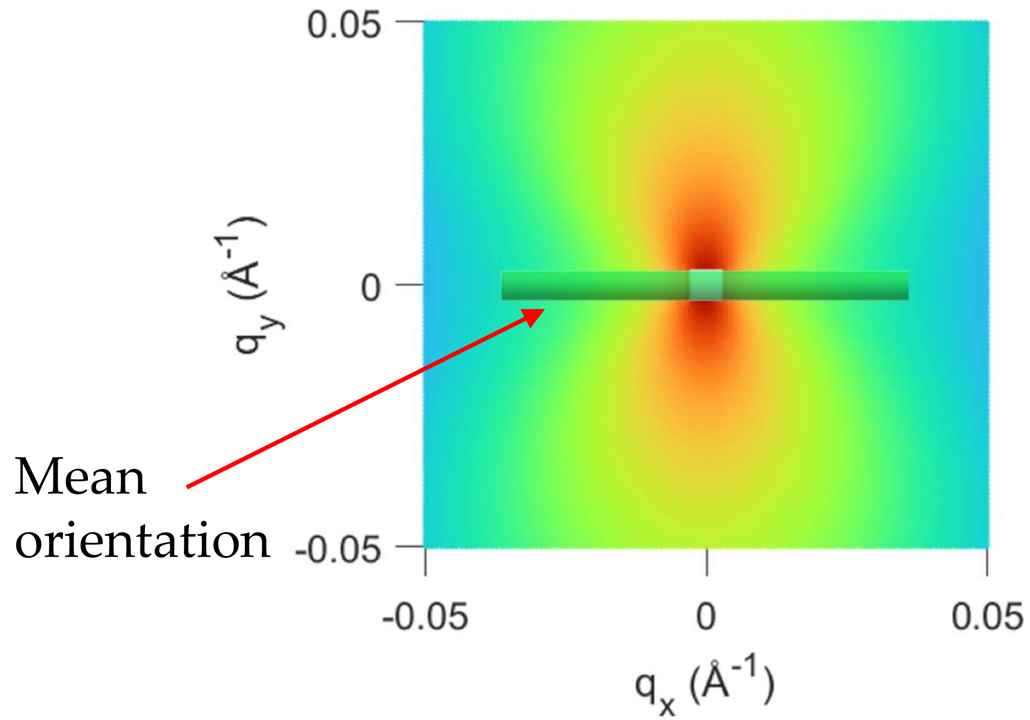


Question:

How do we fit theoretical distribution to experimental data?

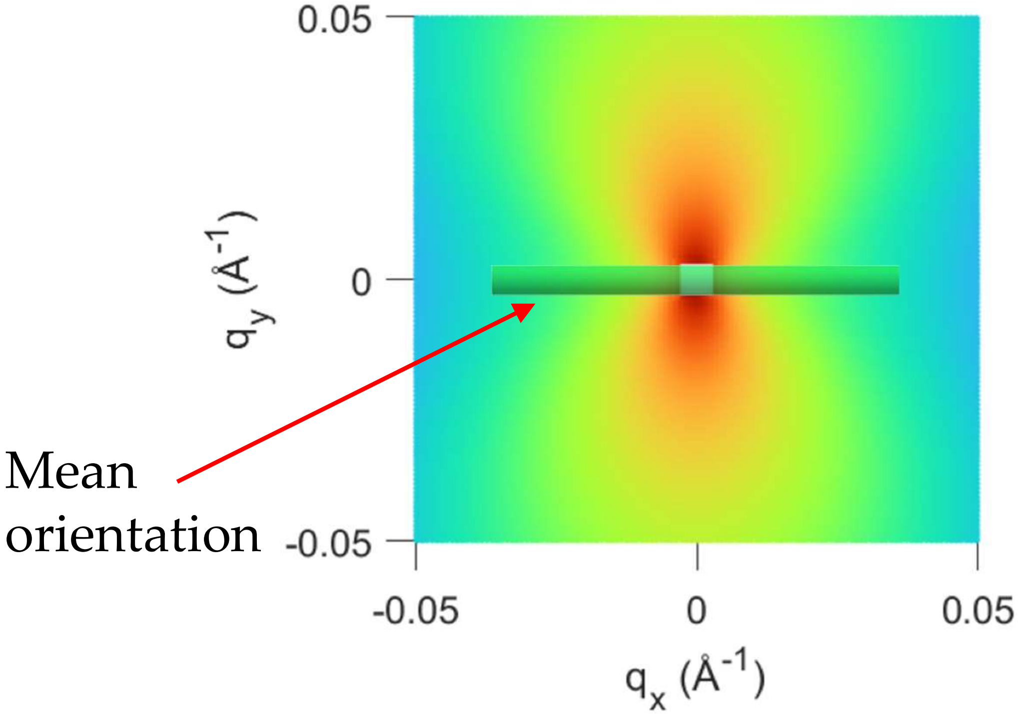


Comparing experimental and theoretical data



Comparing experimental and theoretical data

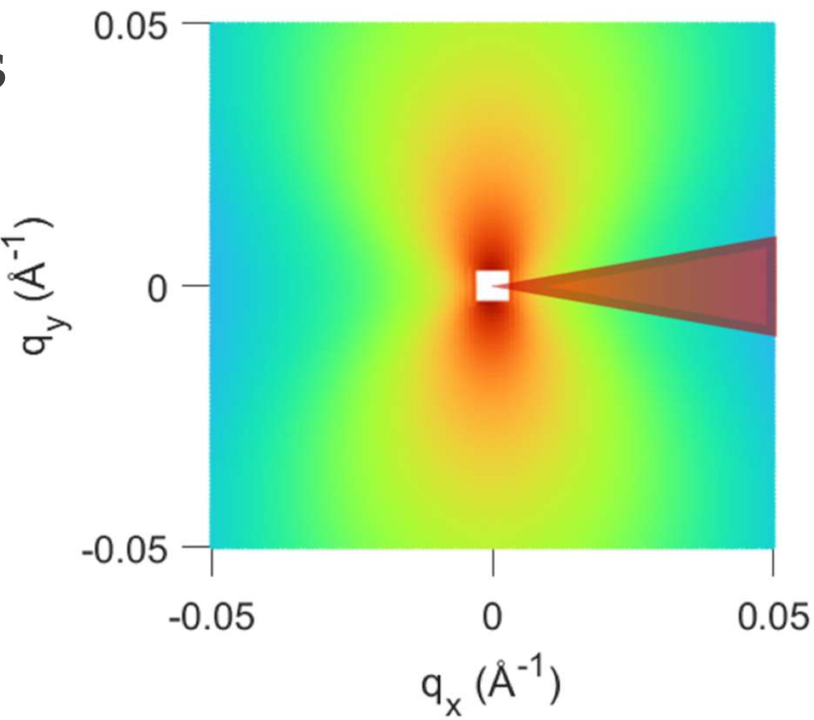
Consider directions perpendicular and parallel to the mean orientation



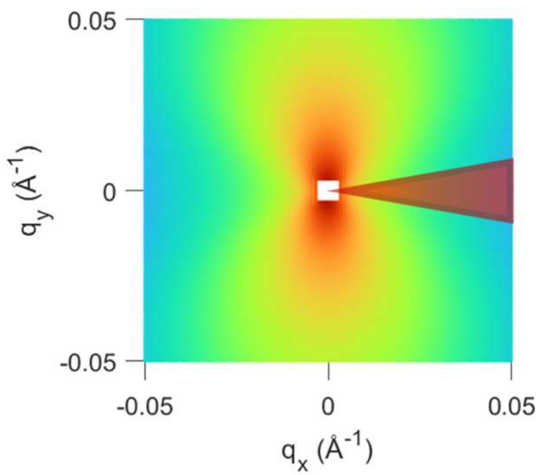
Comparing experimental and theoretical data

Consider directions perpendicular and parallel to the mean orientation

- Perpendicular -> radius
- Parallel -> length



Sector method



Sector method

- Experimental (red)

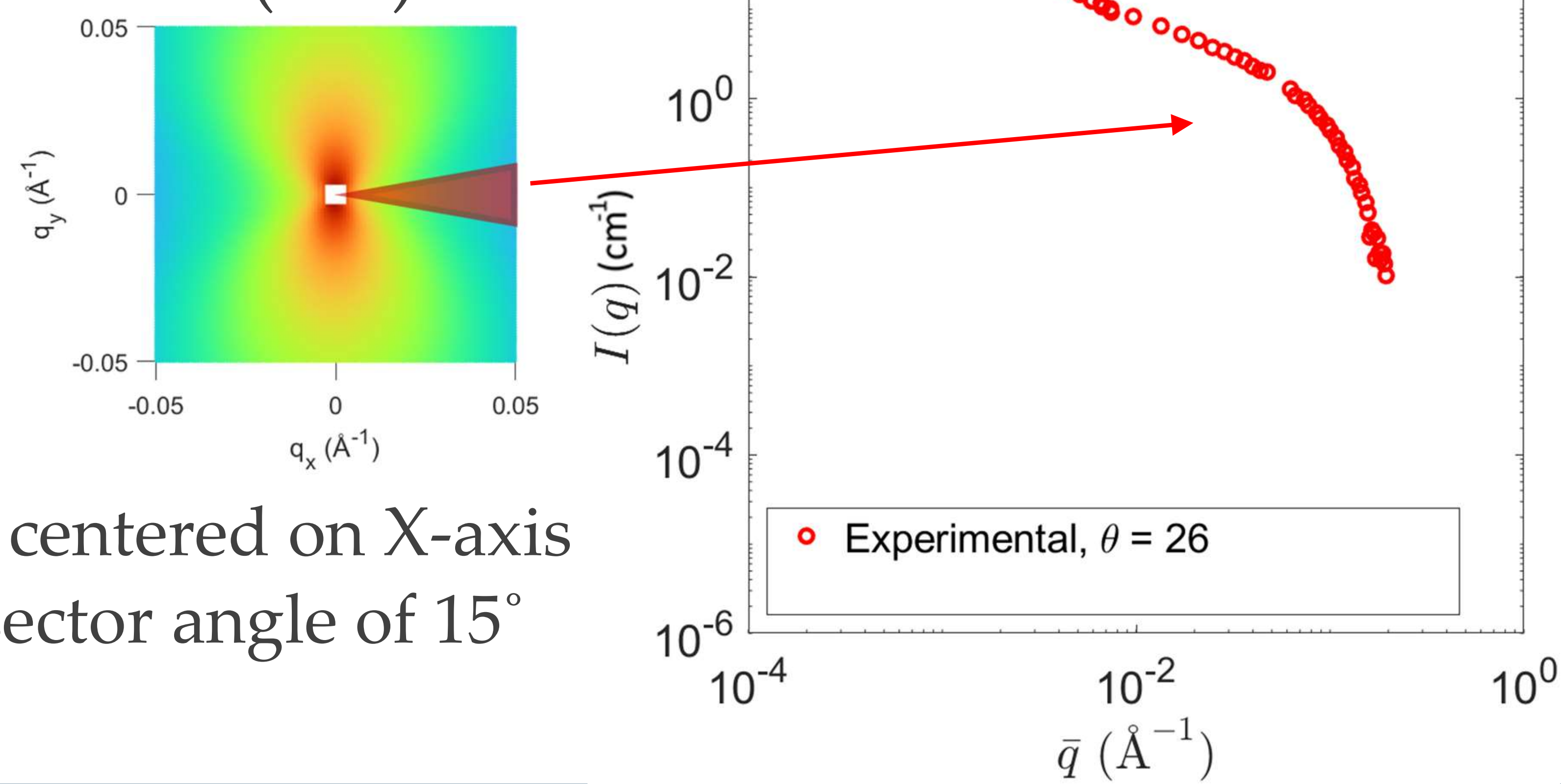


Figure:

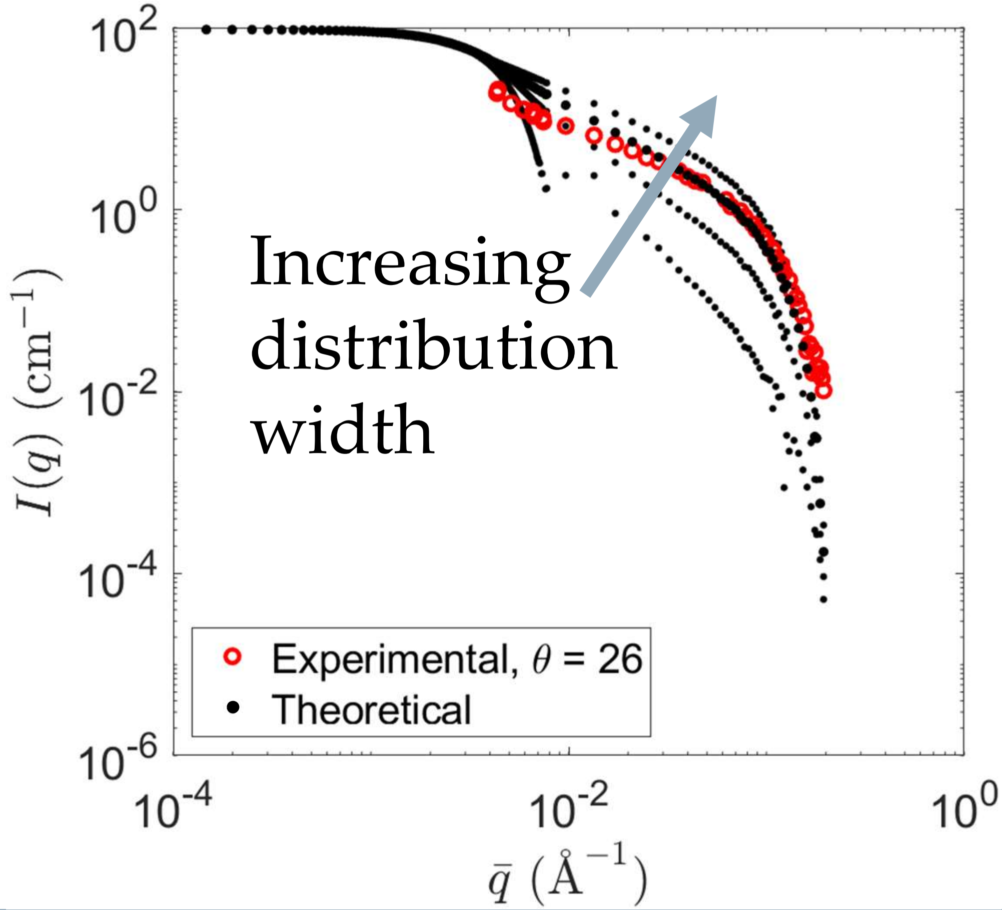
- Sector centered on X-axis
- Total sector angle of 15°

Sector method

- Experimental (red)
- Theoretical (black)

Figure:

- Sector centered on X-axis
- Total sector angle of 15°

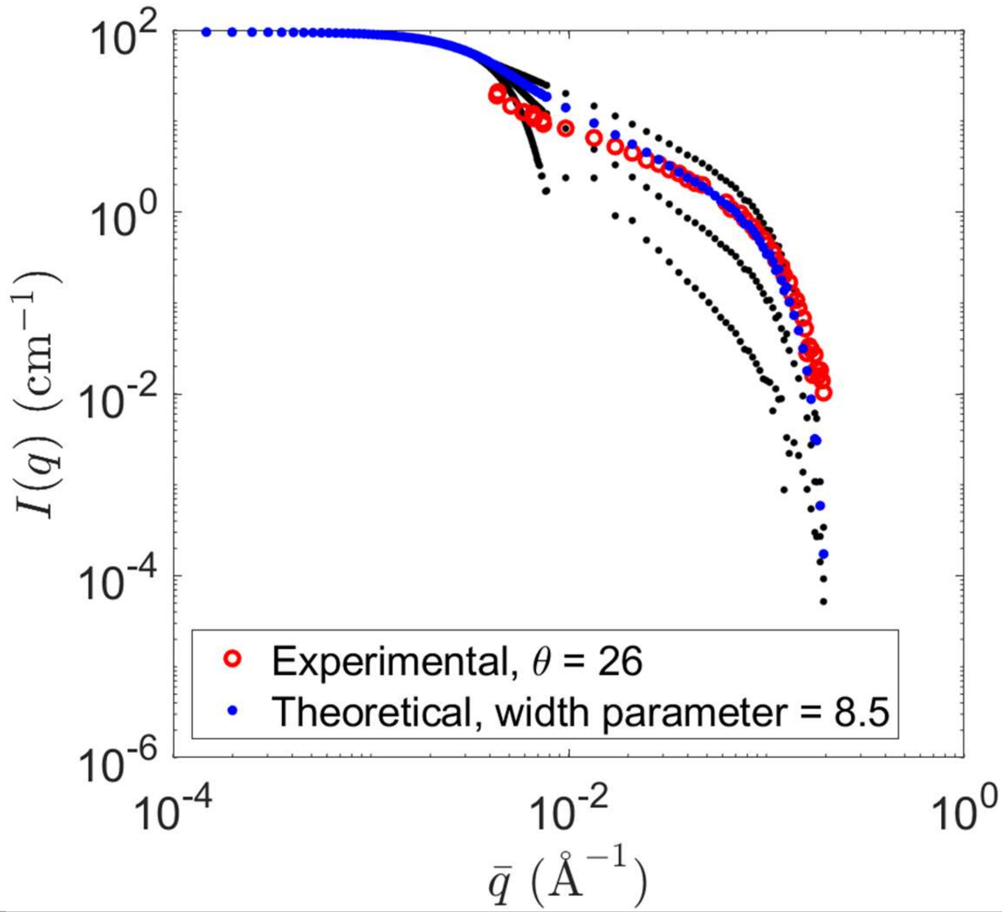


Sector method

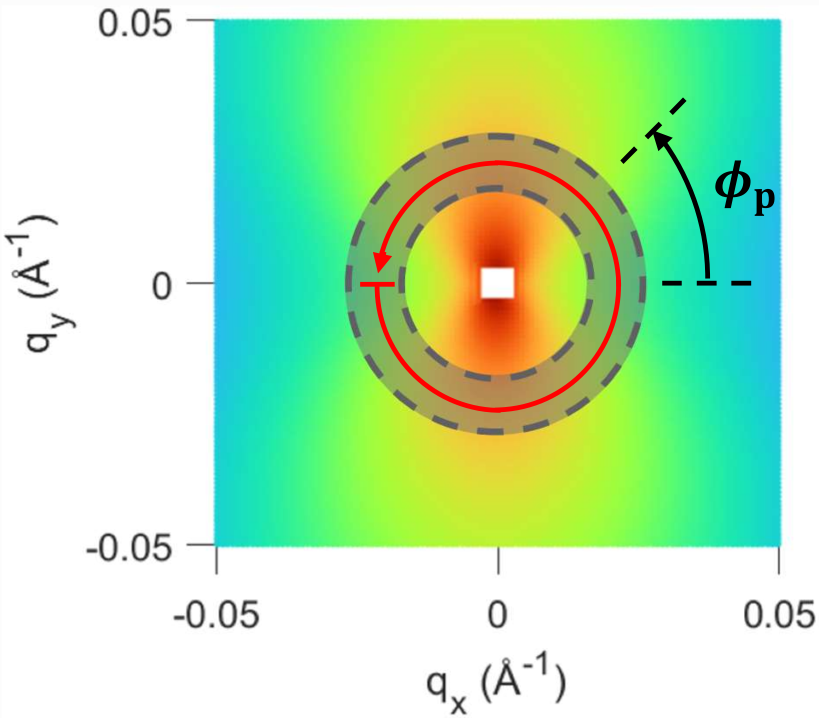
- Experimental (red)
- Theoretical (black)
- Best fitting (blue)

Figure:

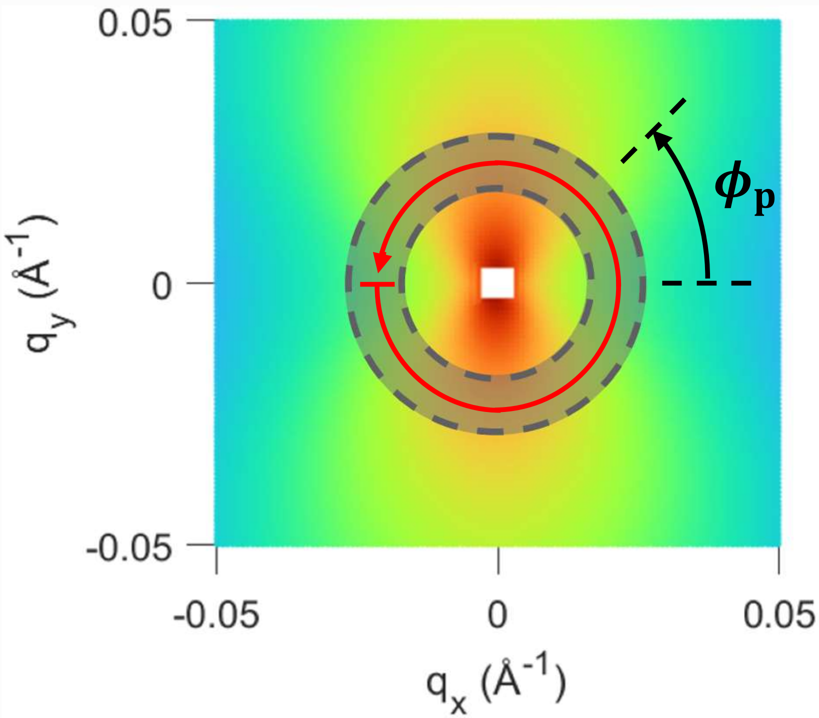
- Sector centered on X-axis
- Total sector angle of 15°

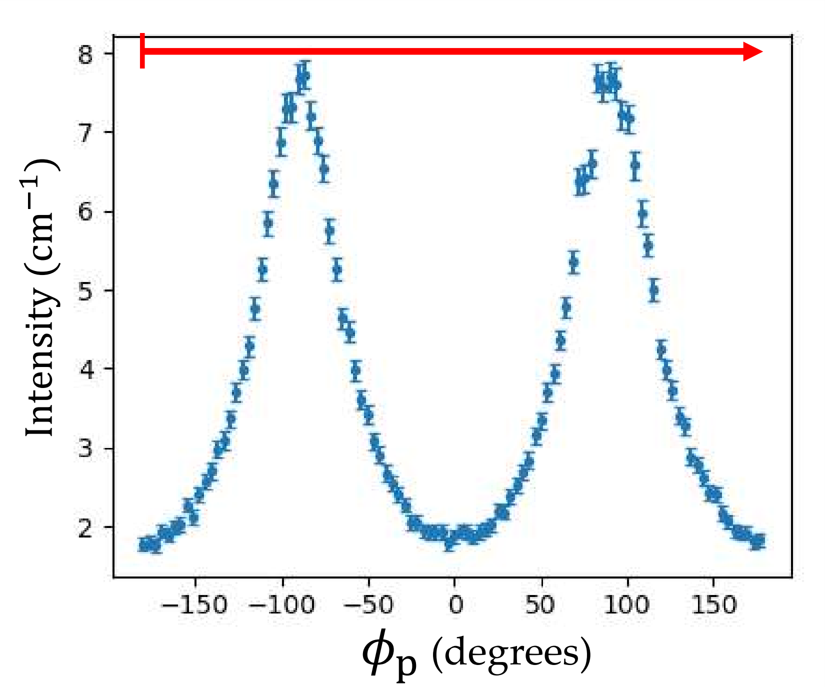


Anisotropy factor method



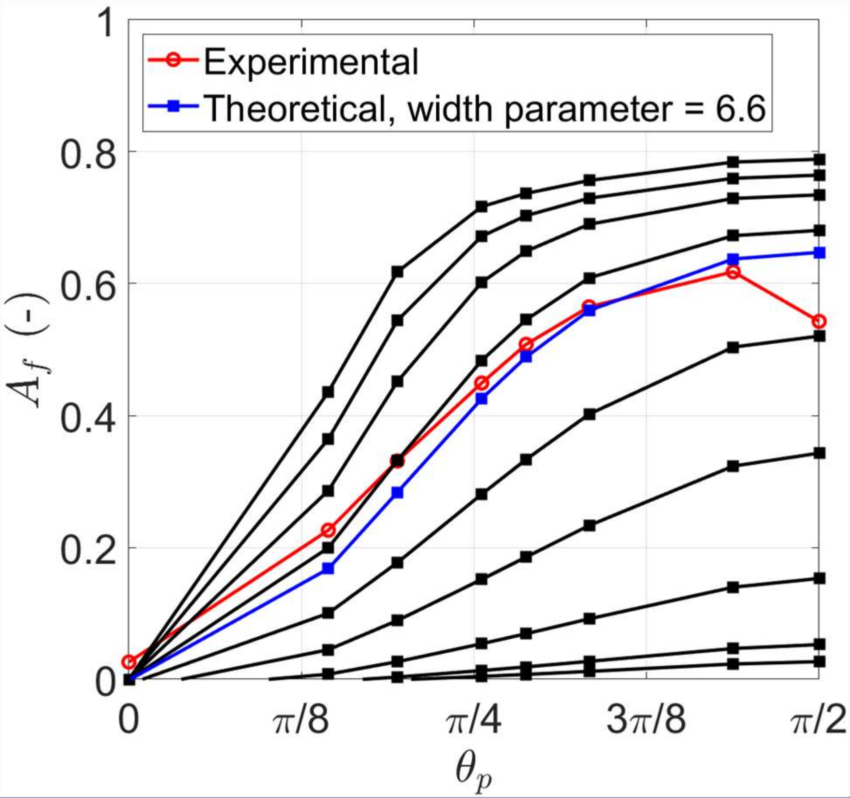
Anisotropy factor method

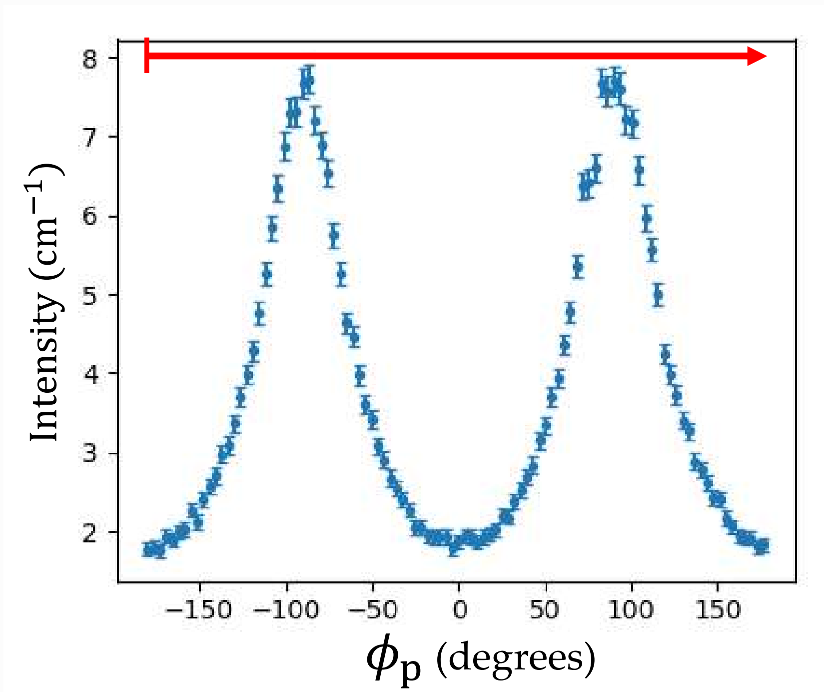




Anisotropy factor method

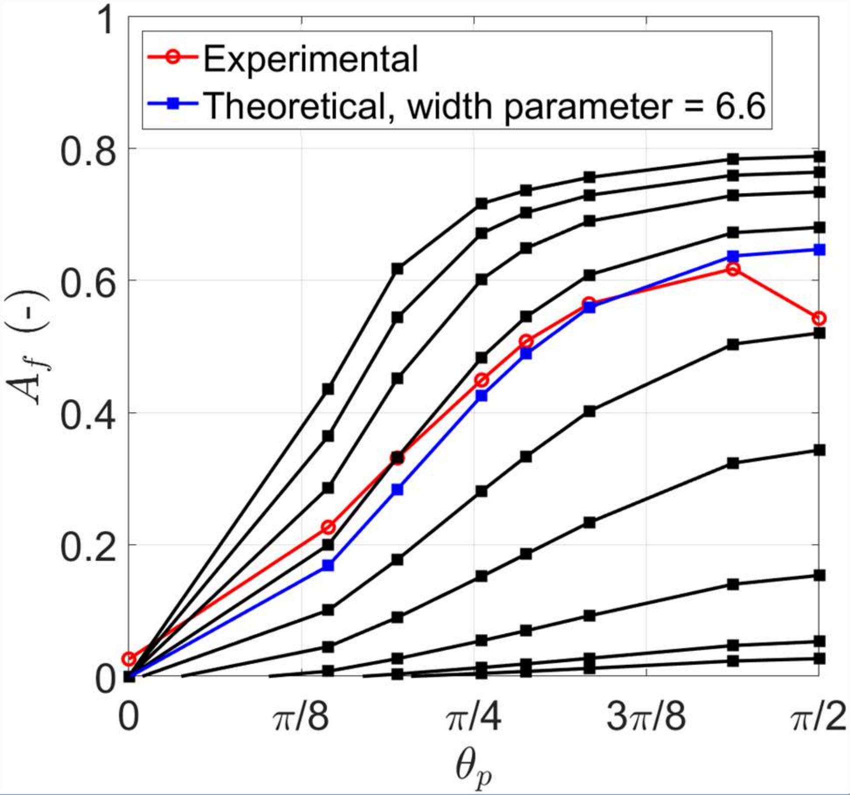
Anisotropy factor



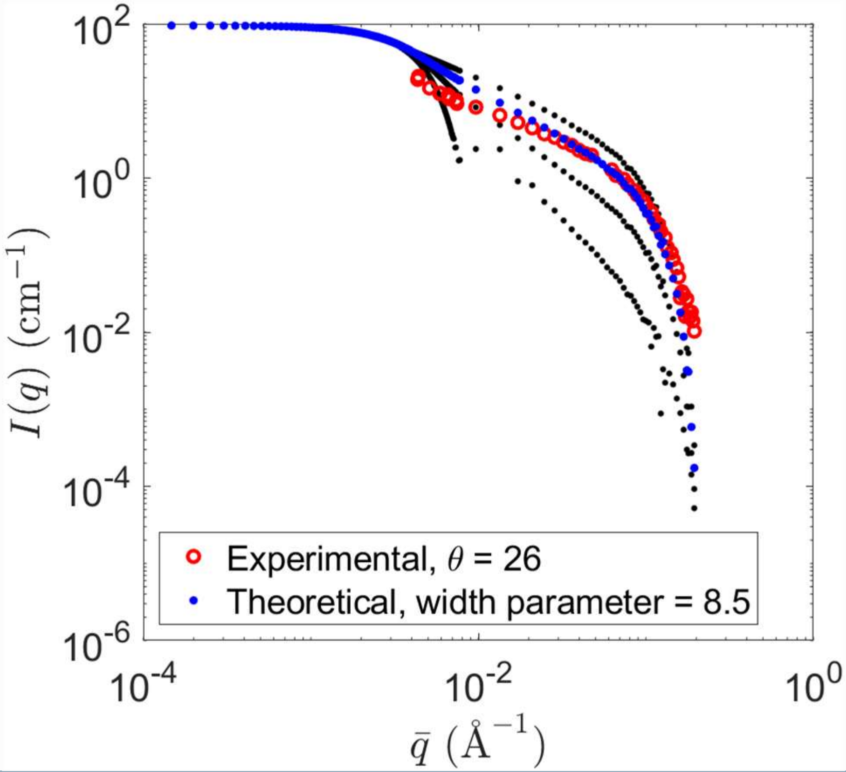


Anisotropy factor method

Anisotropy factor

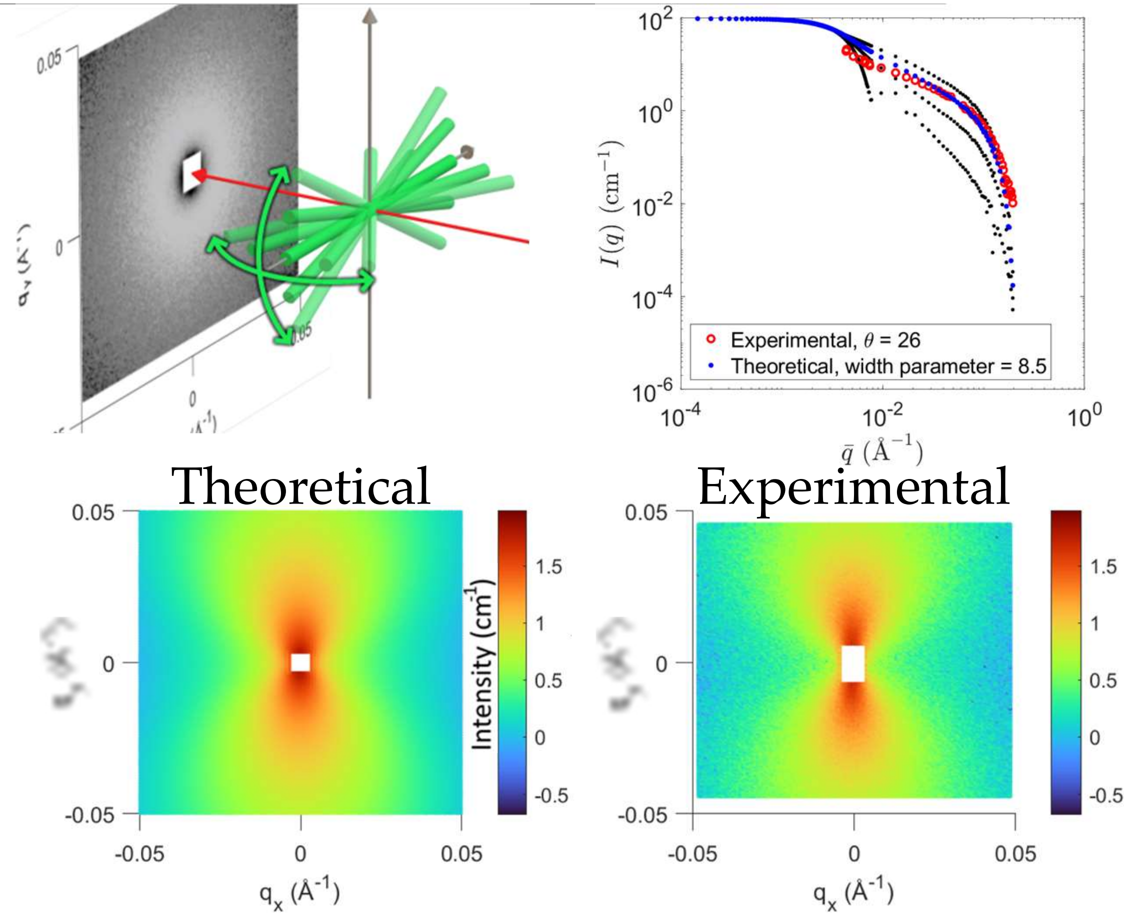


Sector method



Conclusion

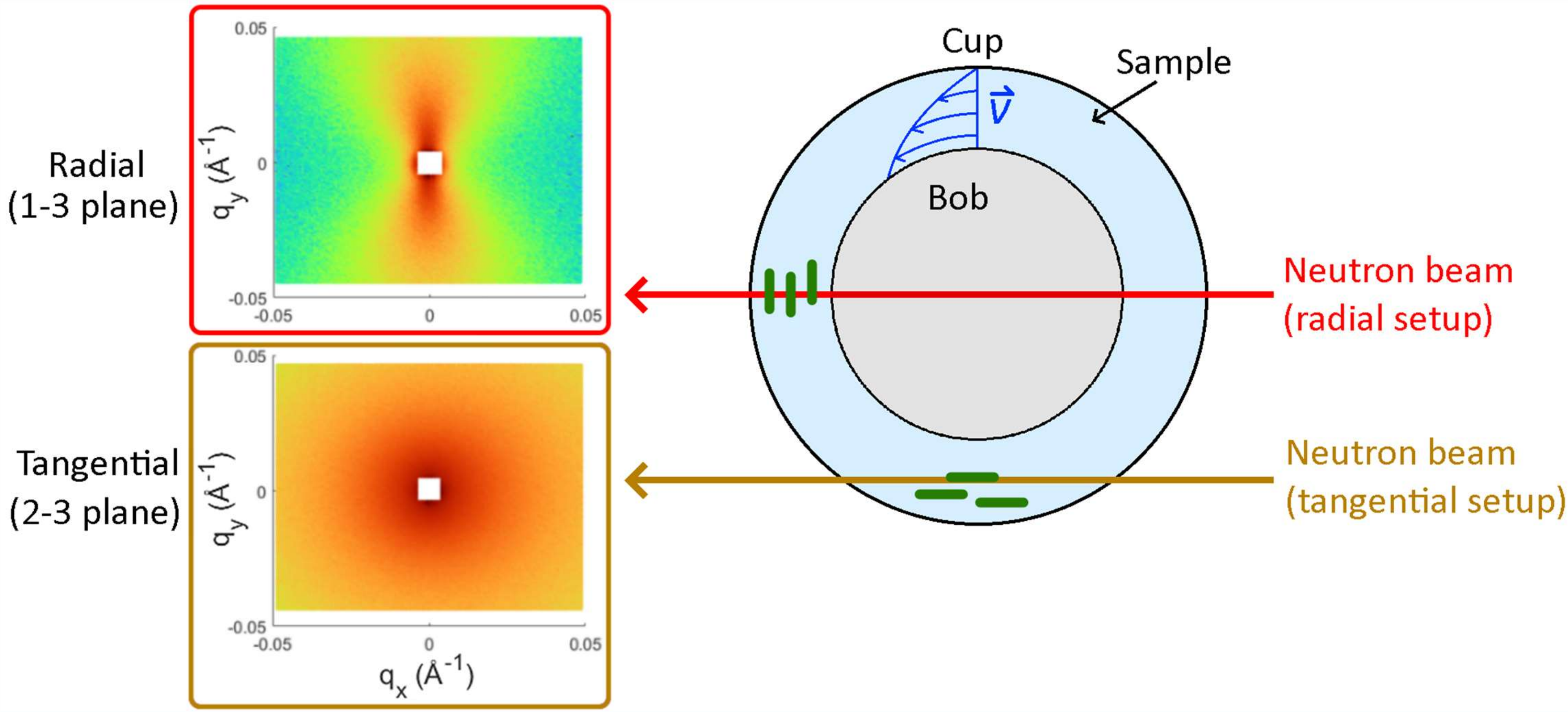
- <u>Orientation distribution</u> can be obtained from small angle neutron scattering
- Can control orientation to design materials



jrooks@udel.edu

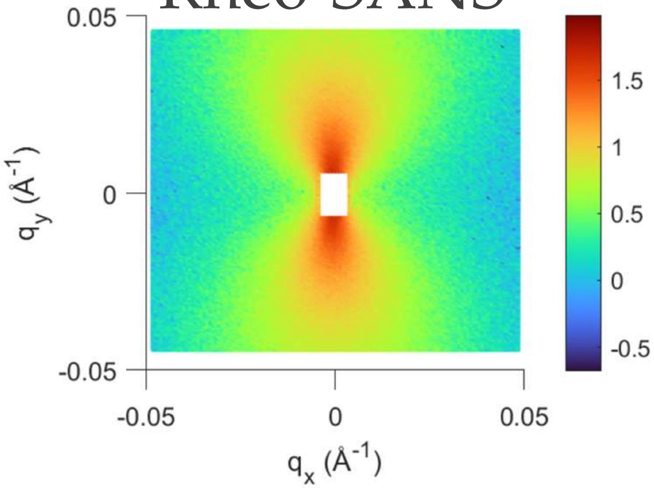
Supplementary slides

Experimental Setup (Rheometer)

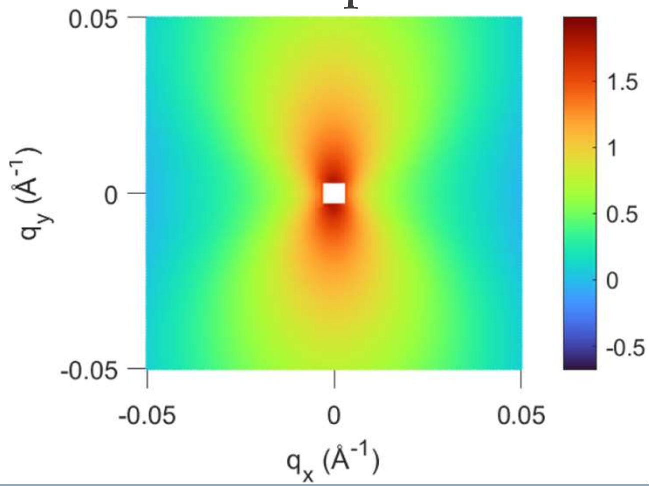


Obtaining data

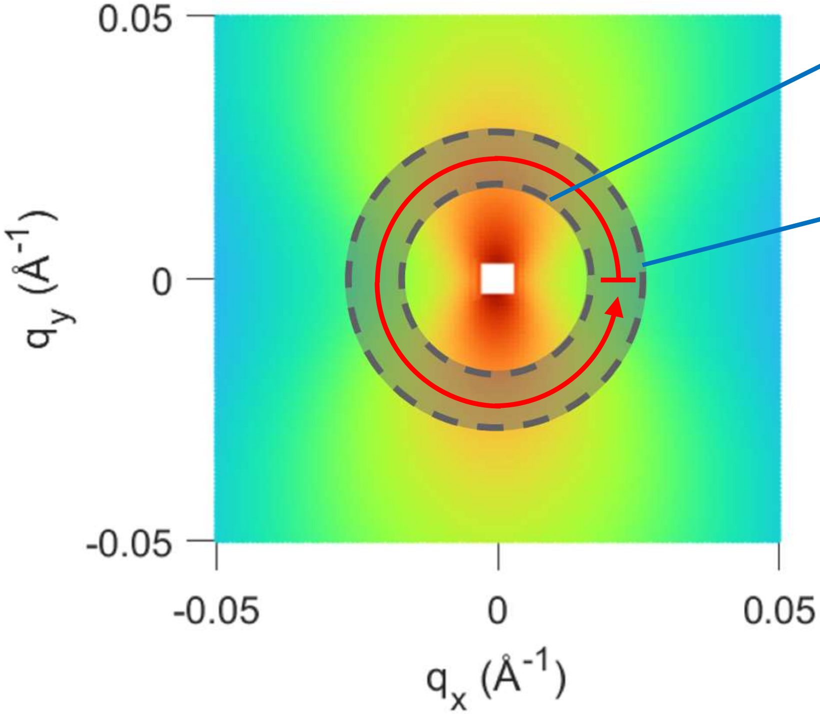
- Experimental (10s^{-1} shear rate)
  - Cylindrical micelles
    - Cetrimonium bromide (CTAB)
  - Rheo-SANS



- Theoretical
  - Cylindrical rods
    - Based on fitting parameters from experimental CTAB



Anisotropy factor – q range



q1 (inner radius) = $\frac{2\pi}{L}$

q2 (outer radius) = $\frac{j_{1,1}}{R}$

with $j_{1,1}$ the first positive 0 of the Bessel function of the first kind (≈3.83)

$$A_{\mathrm{f,cos}}(q) = \frac{\int_0^{2\pi} I(q,\phi_\mathrm{s}) \cos 2\left(\phi_\mathrm{s} - \phi_{\mathrm{s},0}\right) d\phi_\mathrm{s}}{\int_0^{2\pi} I(q,\phi_\mathrm{s})\, d\phi_\mathrm{s}}$$