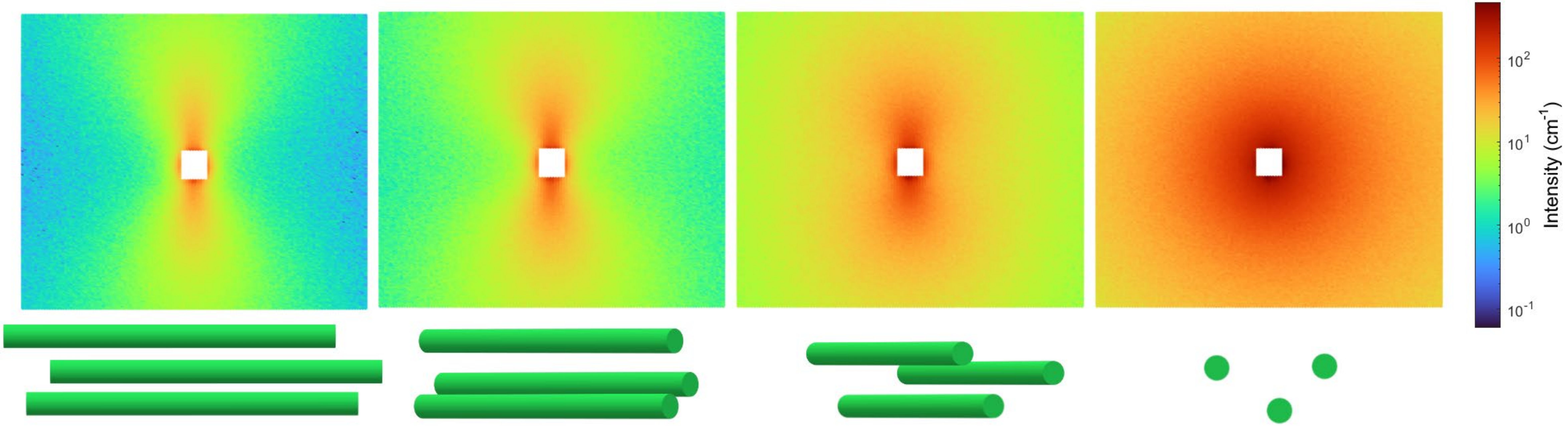
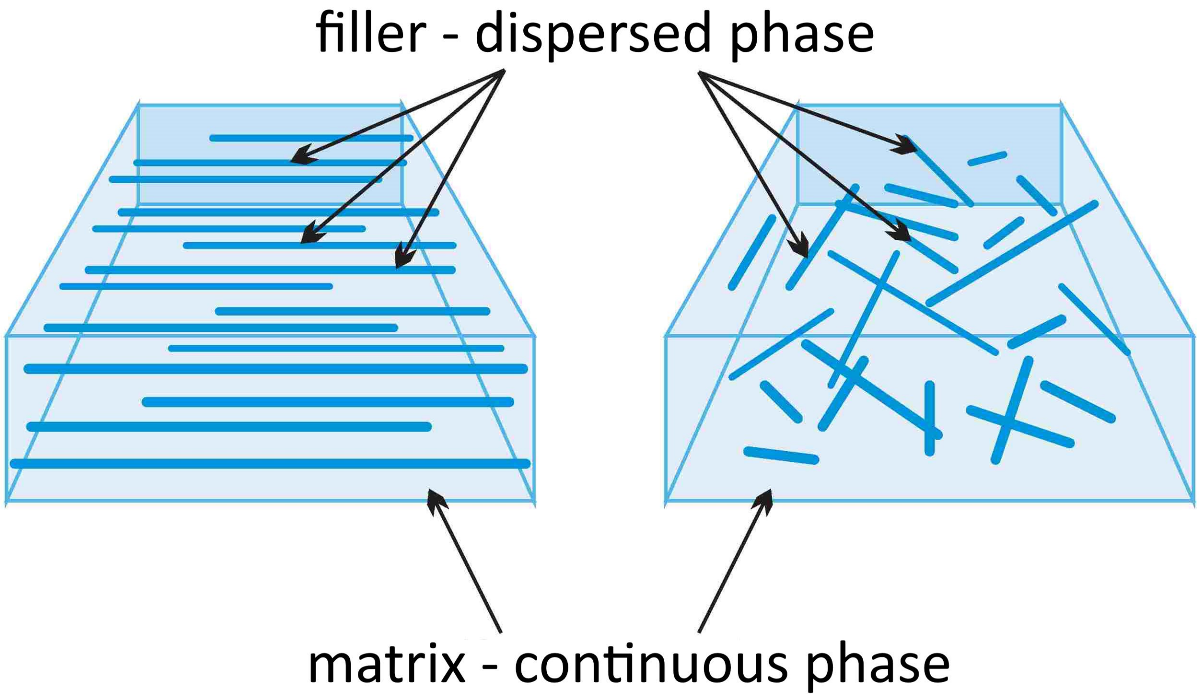
Assessing particle orientation in small angle neutron scattering

Jack Rooks (jackrook@buffalo.edu), Peter Gilbert



Motivation

- Material properties depend on orientation/alignment



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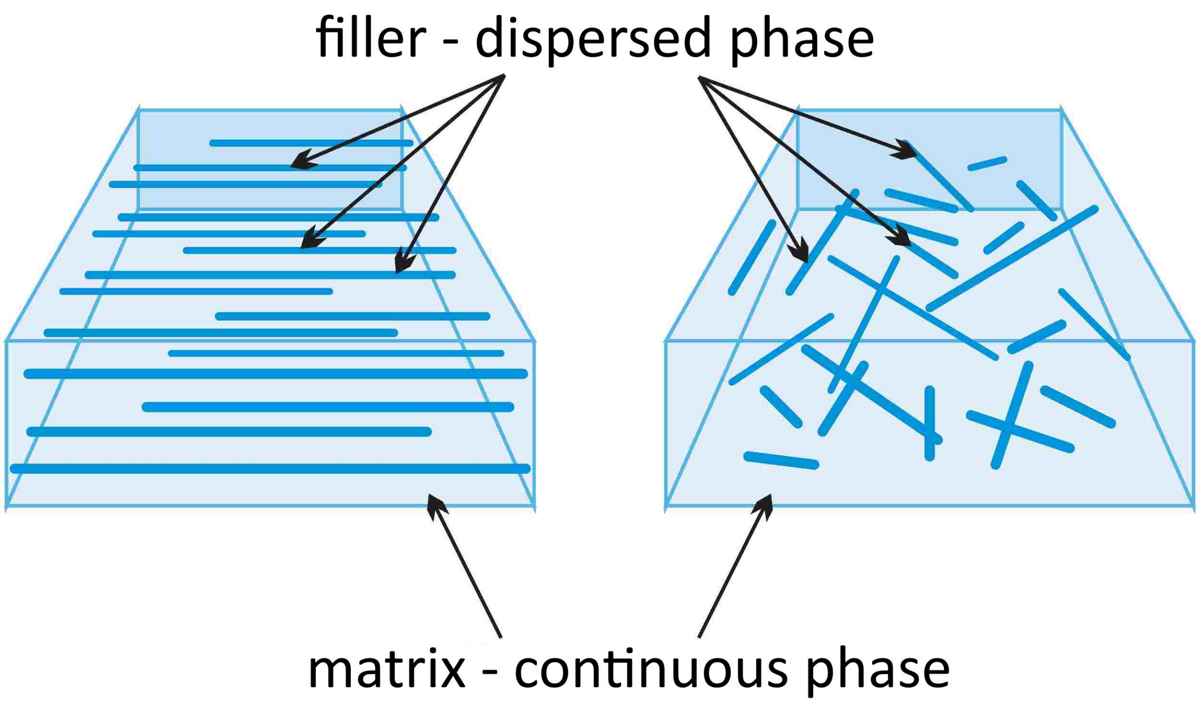

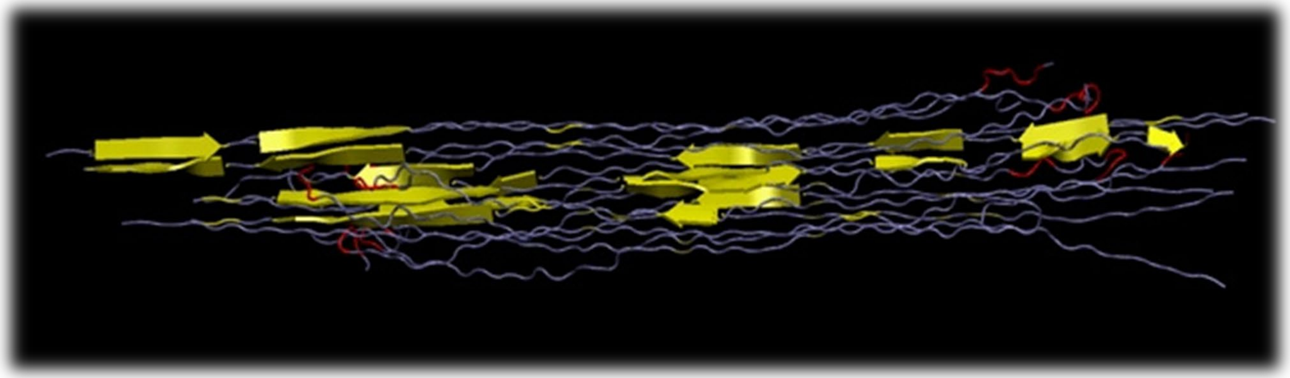

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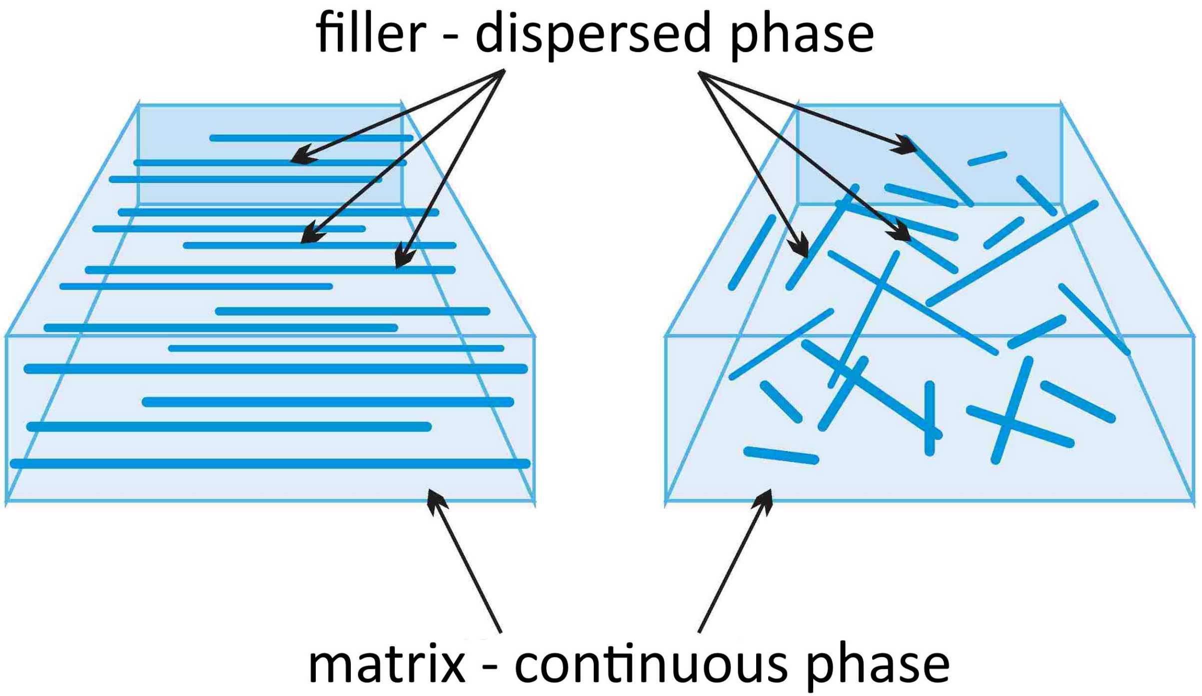
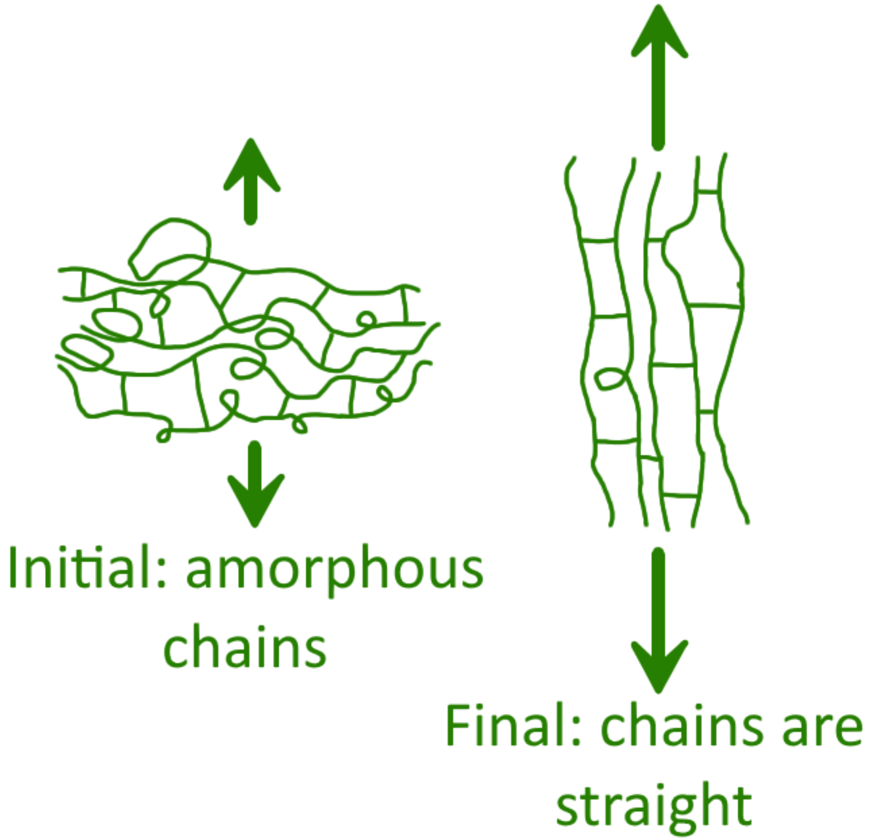
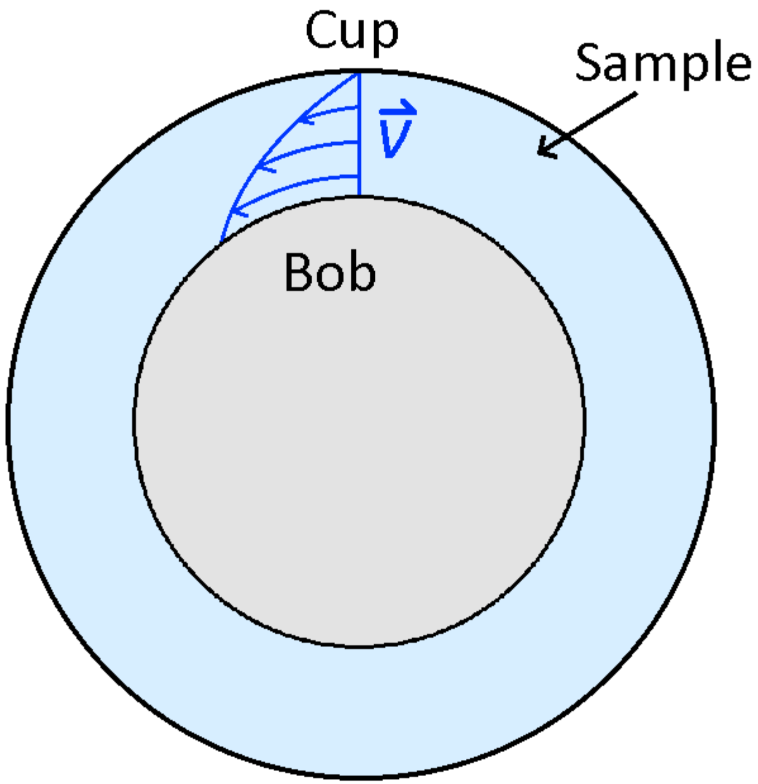




https://www.slideserve.com/malo/chapter-15-polymers-characteristics-applications-and-processing
https://www.essentialchemicalindustry.org/materials-and-applications/composites.html

Experimental Setup (Rheometer)



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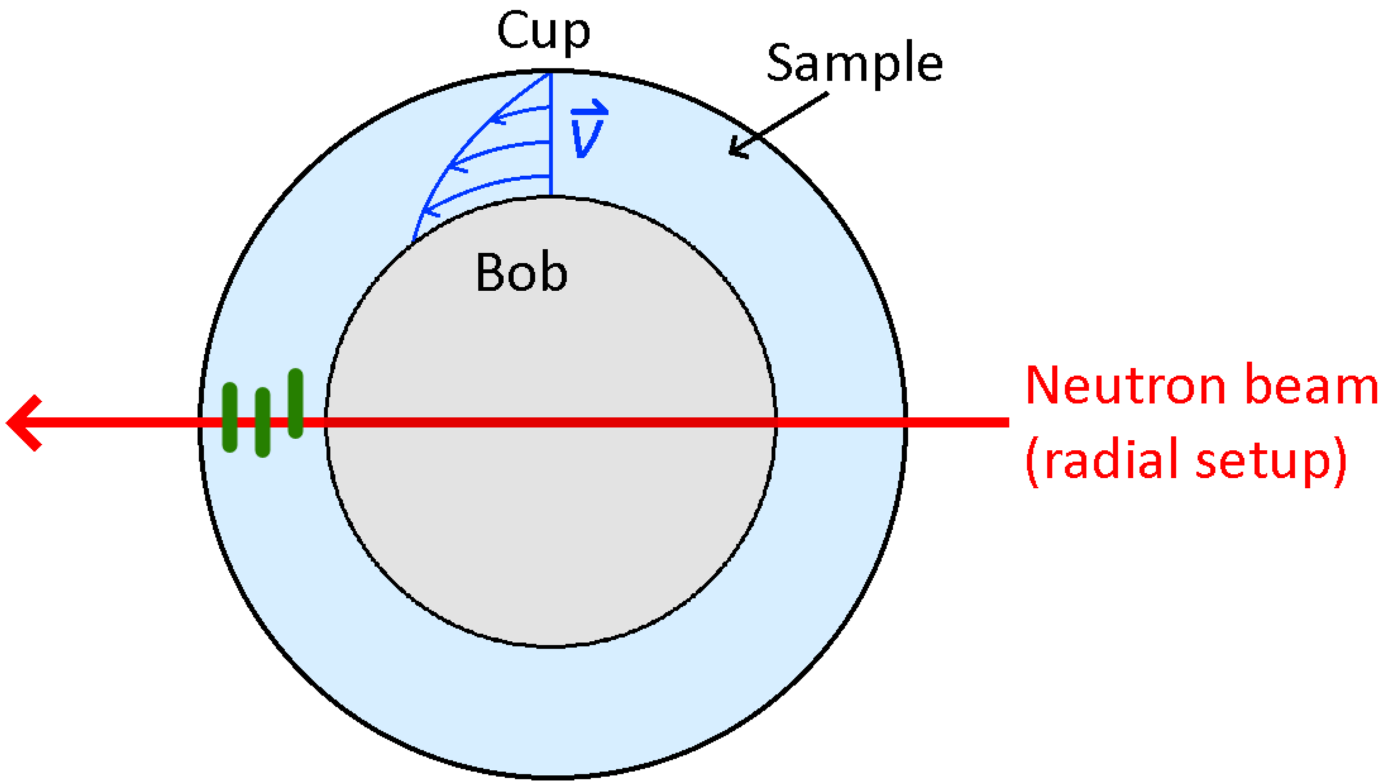
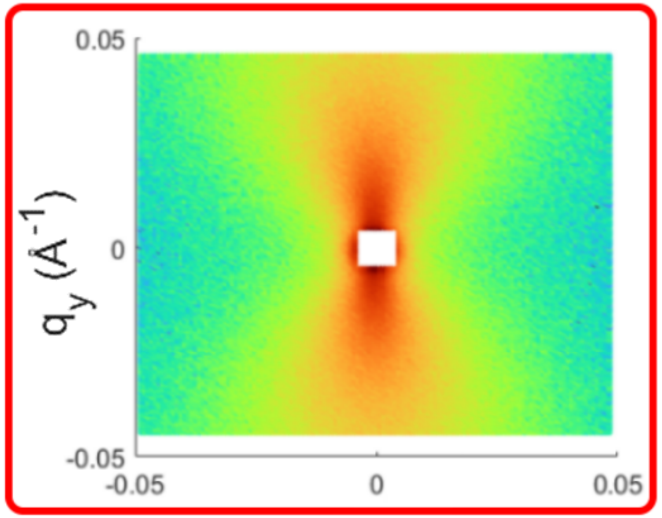
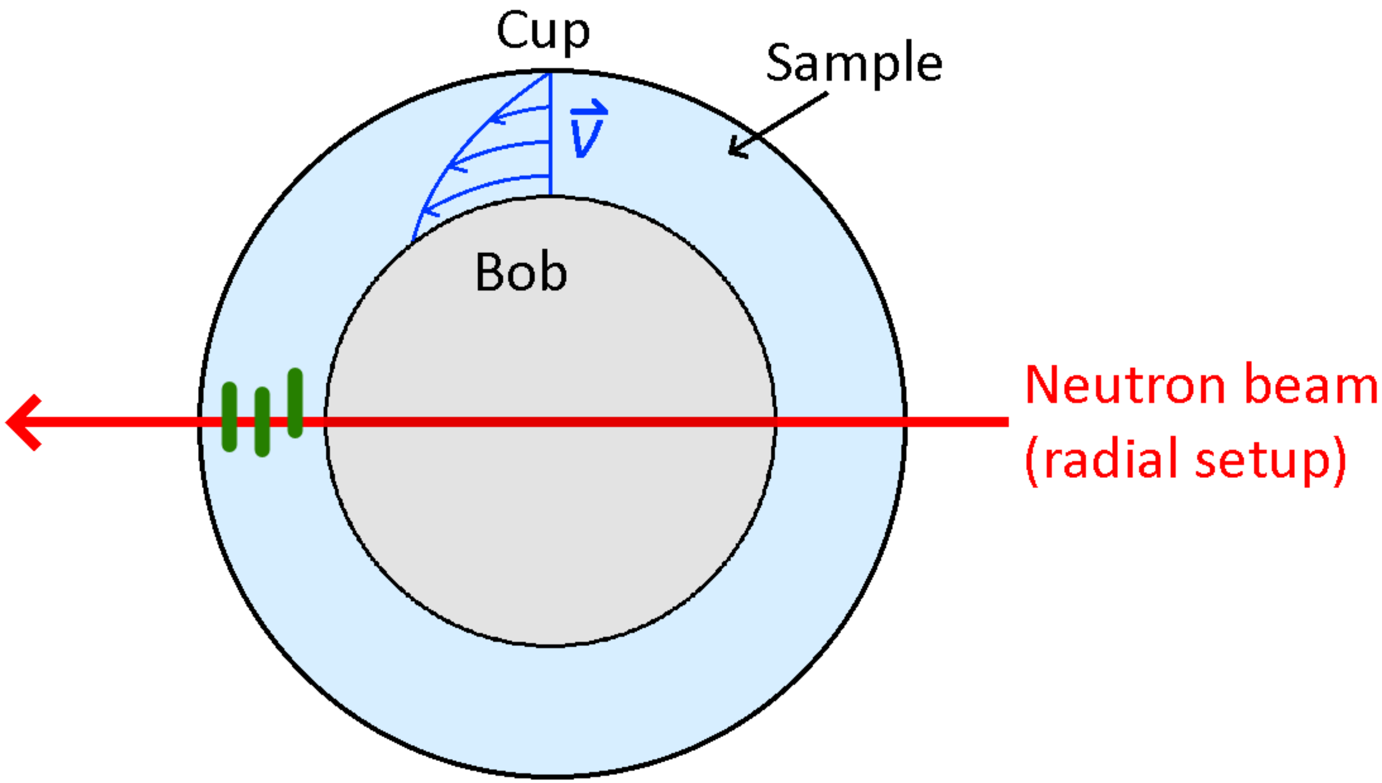


Experimental Setup (Rheometer)

Radial
(1-3 plane)





Experimental Setup (Rheometer)

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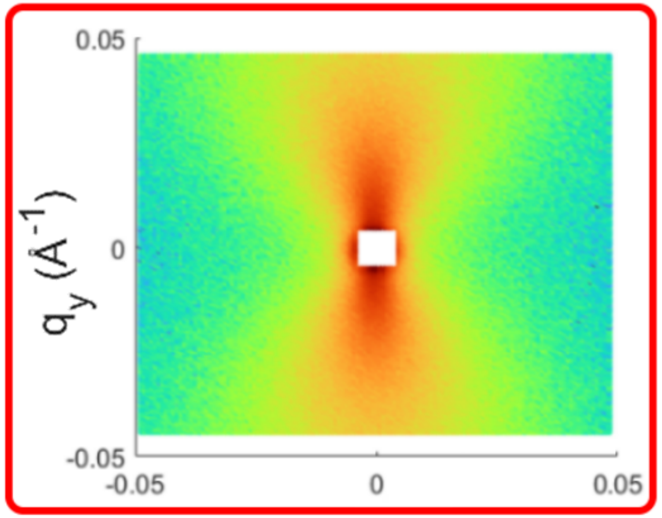
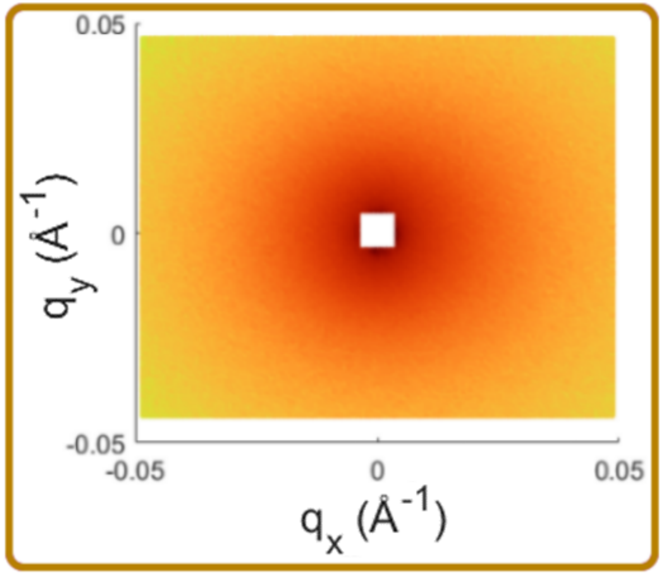
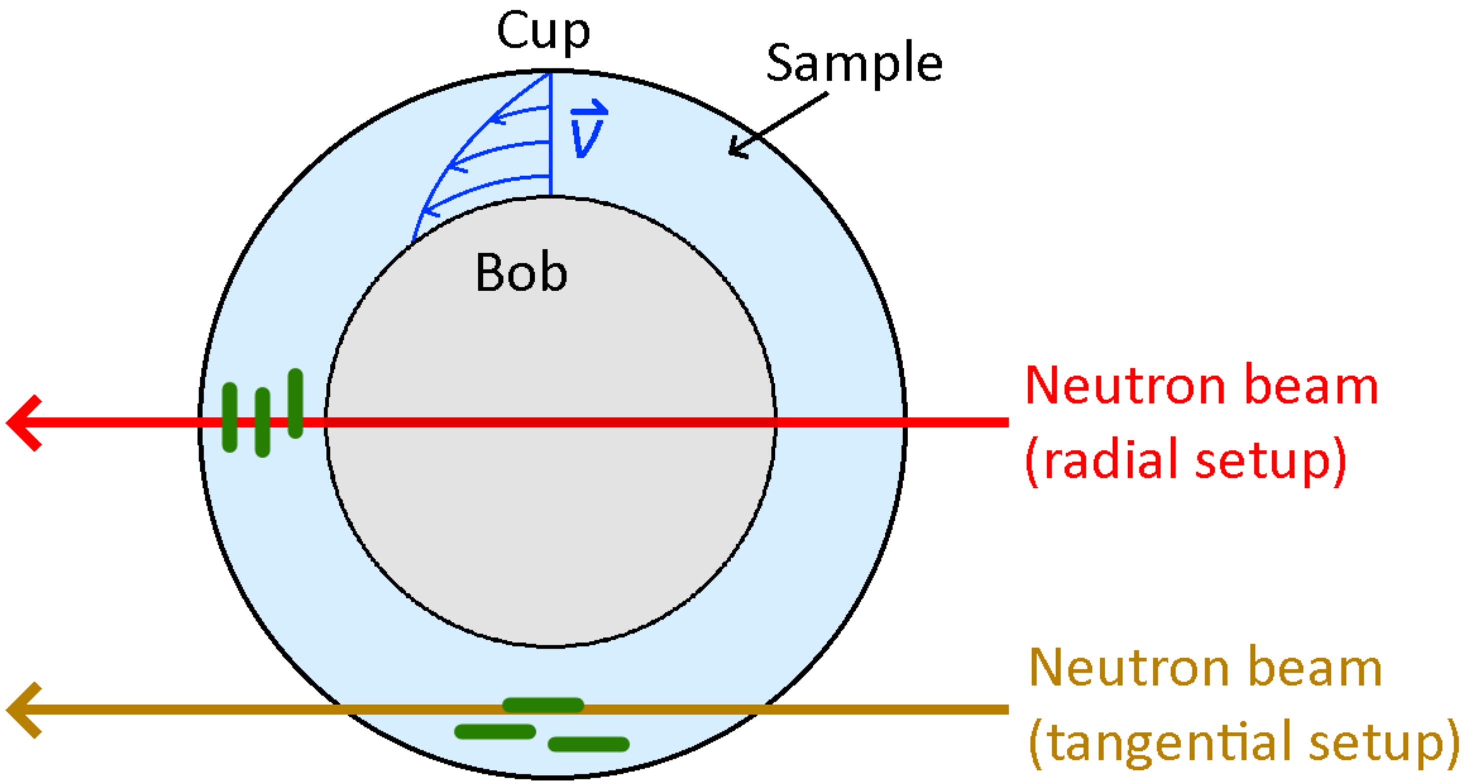
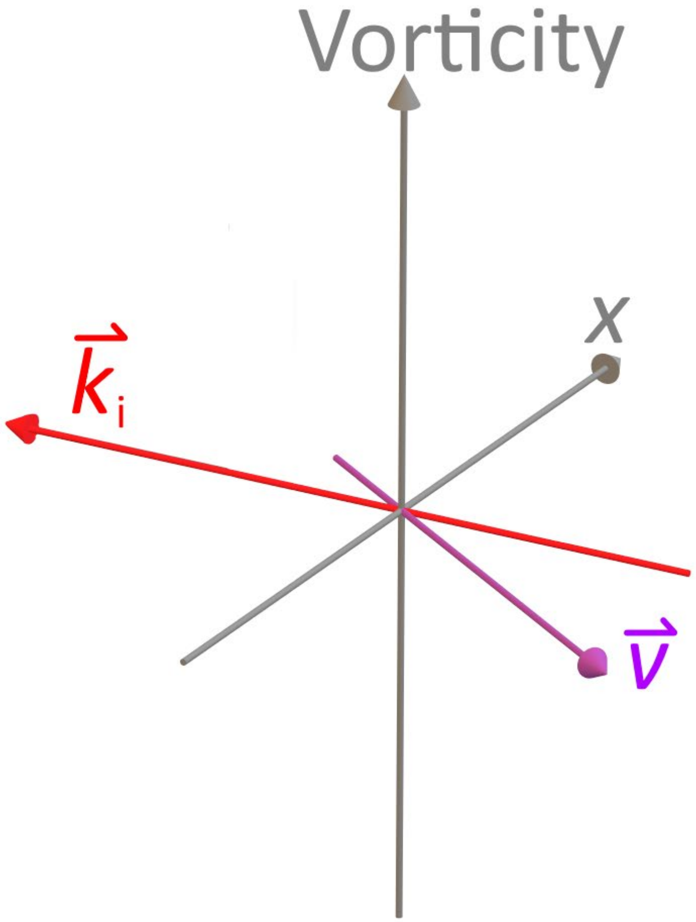


Tangential
(2-3 plane)



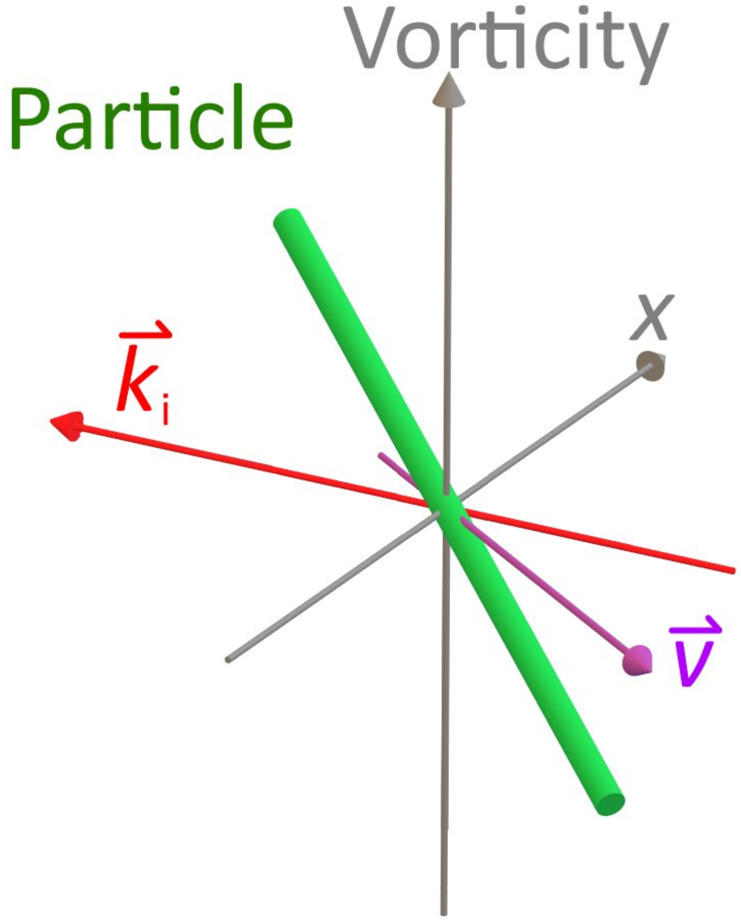


Neutron Scattering



$\vec{k}_i$ - Neutron beam

Neutron Scattering



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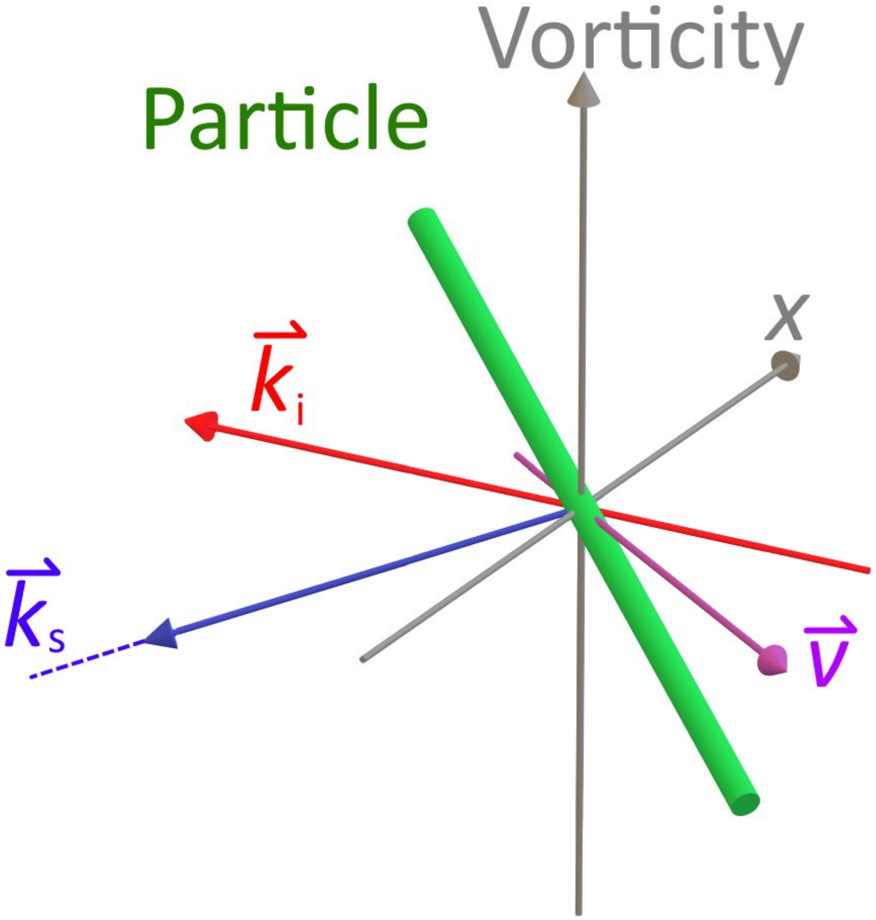
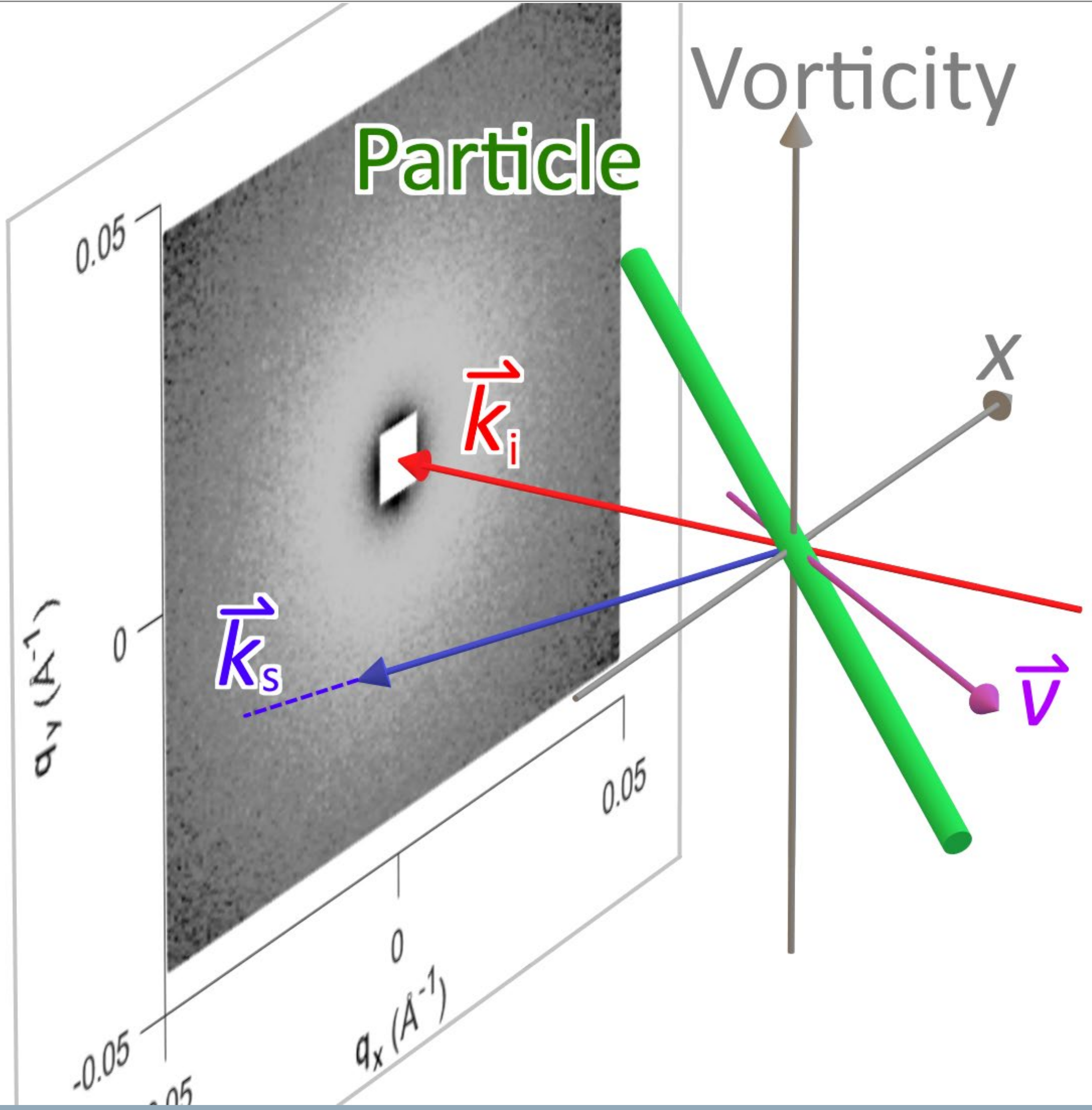


$\vec{k}_i$ - Neutron beam

$\vec{k}_s$ - Scattered neutron

Neutron Scattering



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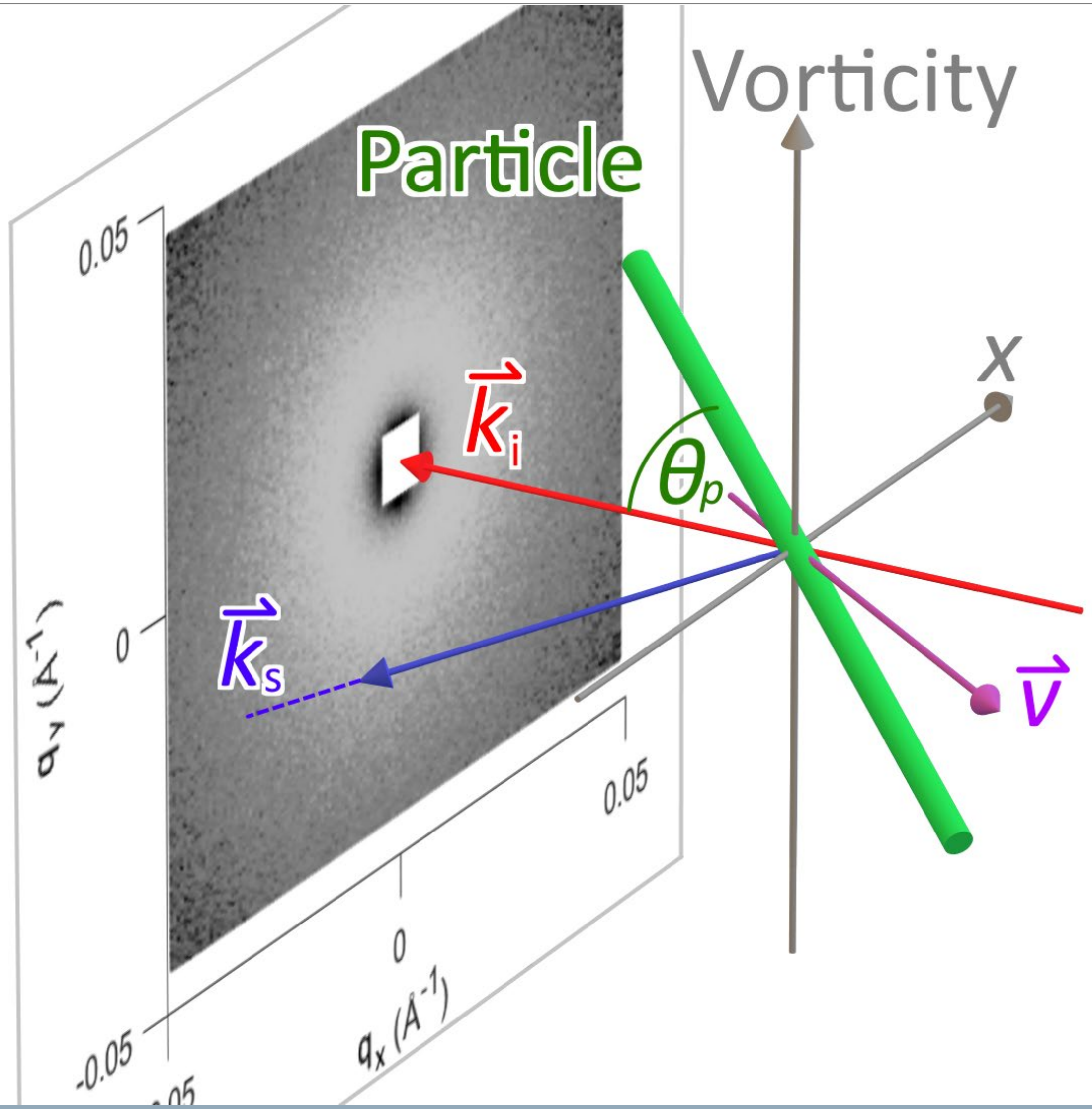
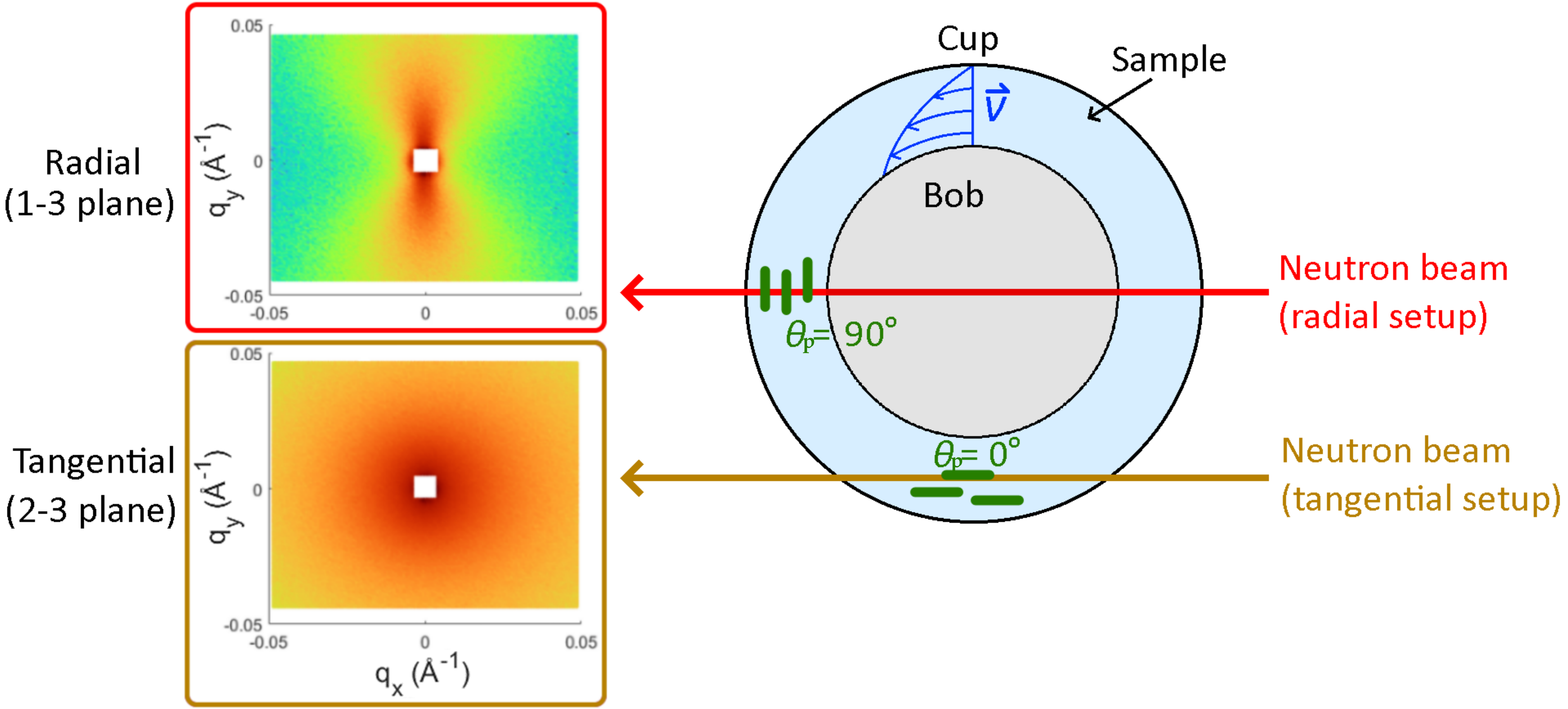


$\vec{k}_i$ - Neutron beam

$\vec{k}_s$ - Scattered neutron

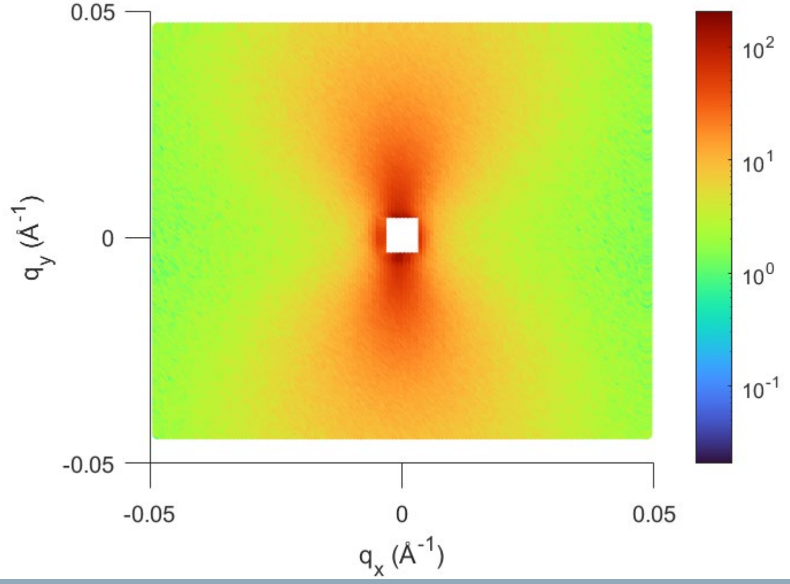
Experimental Setup (Rheometer)



Obtaining Data

Experimental

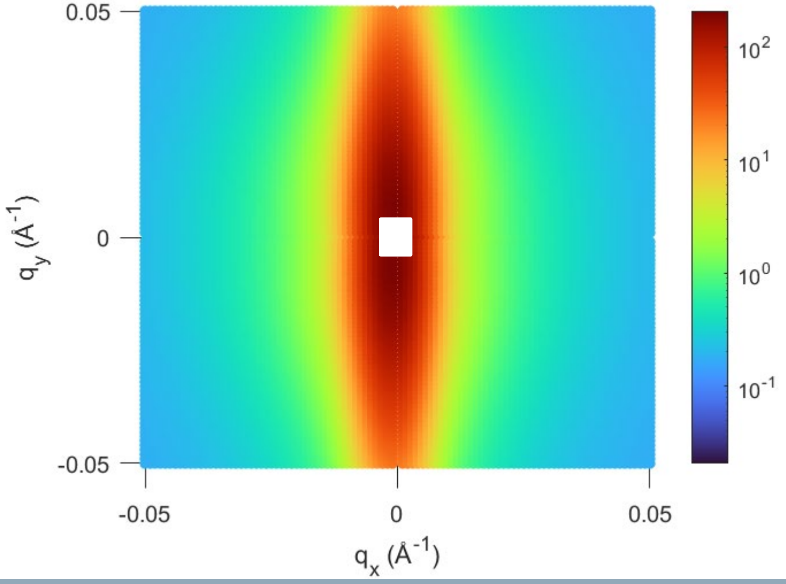
- Cylindrical micelles
  - 0.03 M Cetrimonium bromide (CTAB)
  - 0.24 M Sodium salicylate
- Rheo-SANS
  - 10 s^{-1} shear rate



Obtaining Data

Theoretical

- Cylindrical rods
  - Mean radius of 20 Å
  - 5% polydispersity in radius
  - Length of 1800 Å



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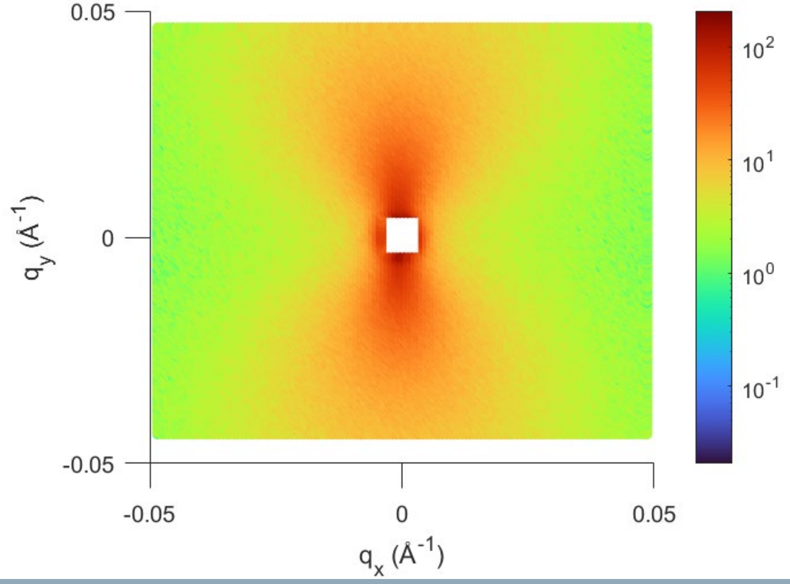
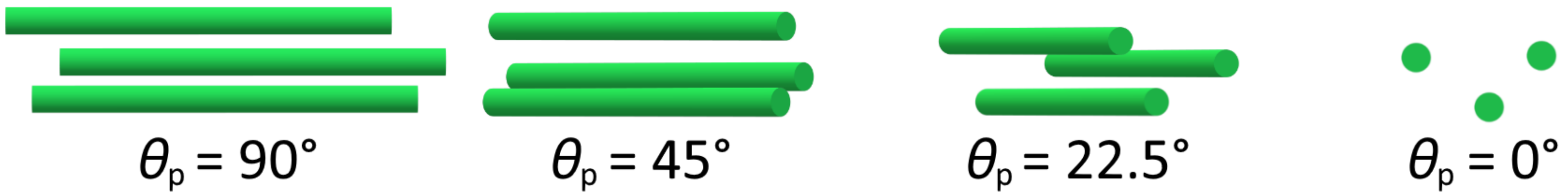


Characterizing Alignment



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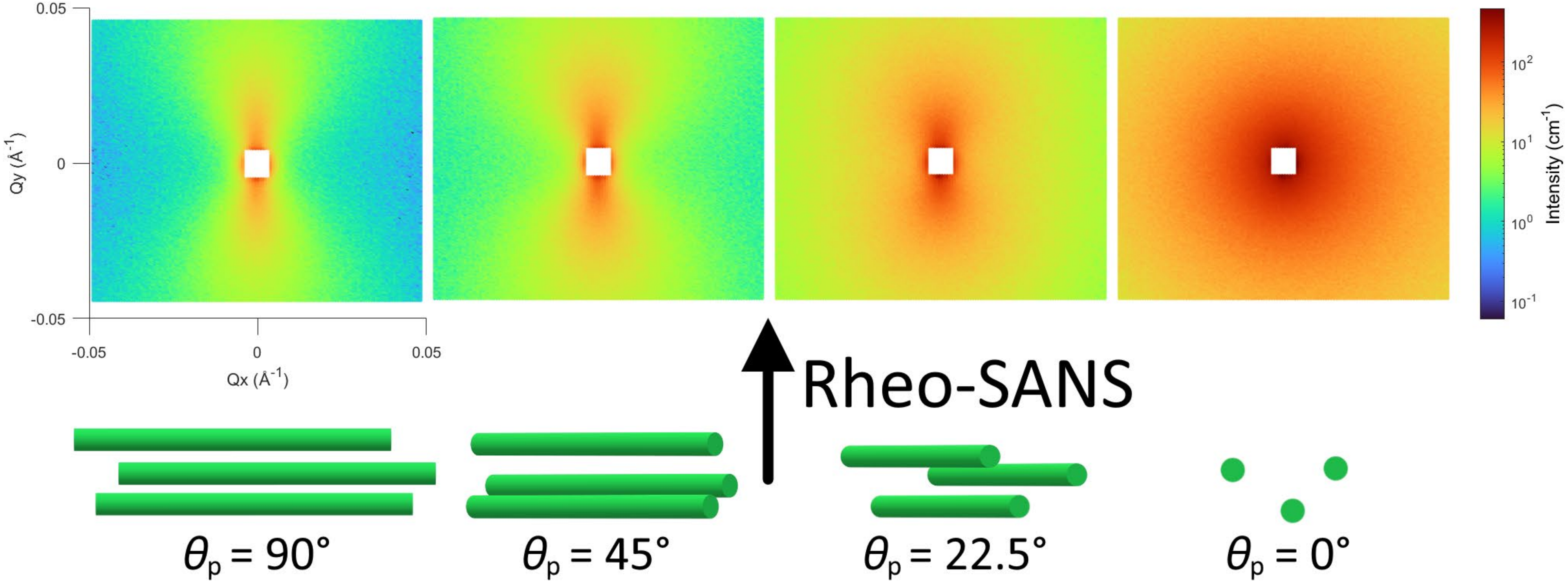

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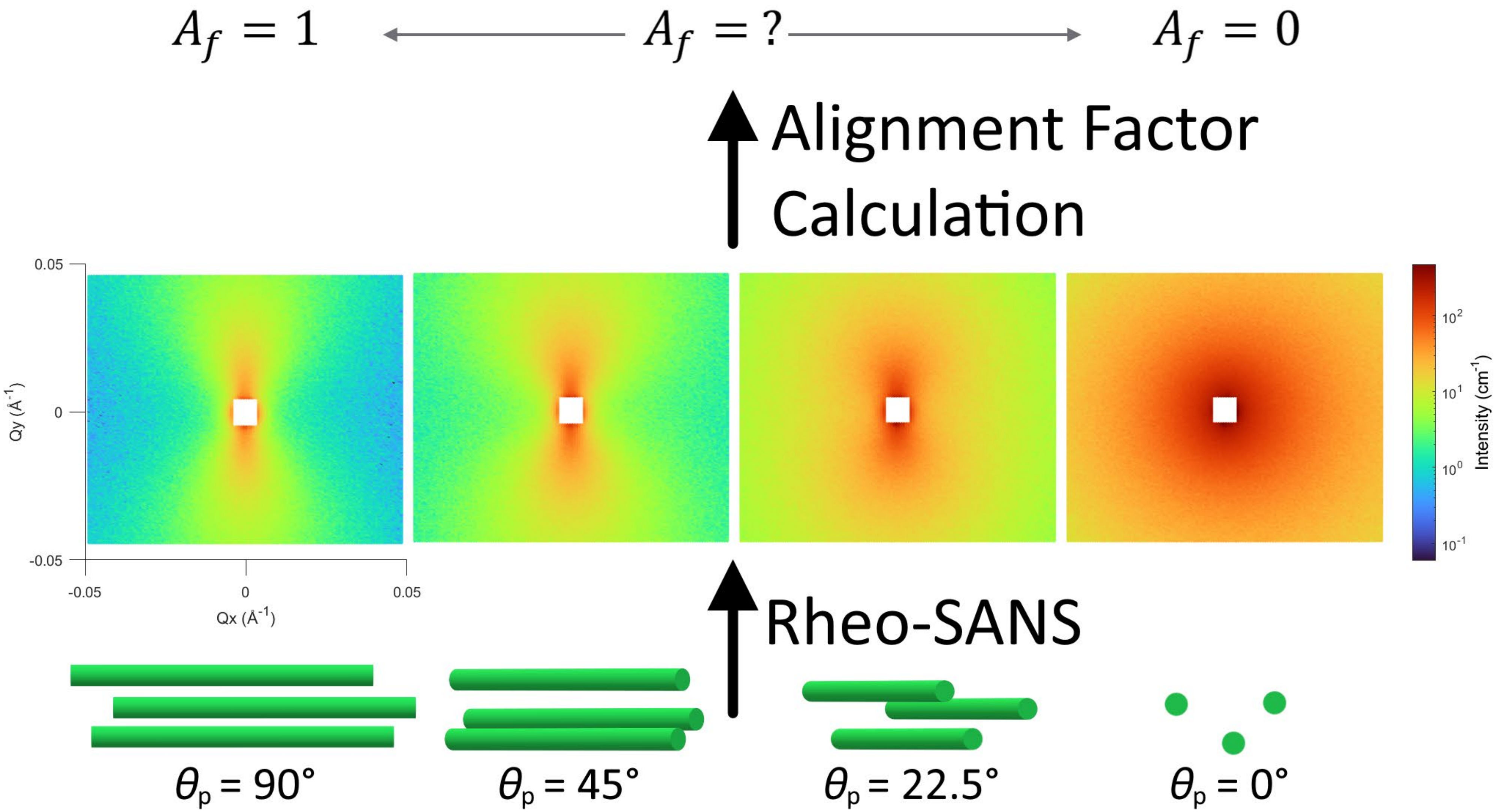

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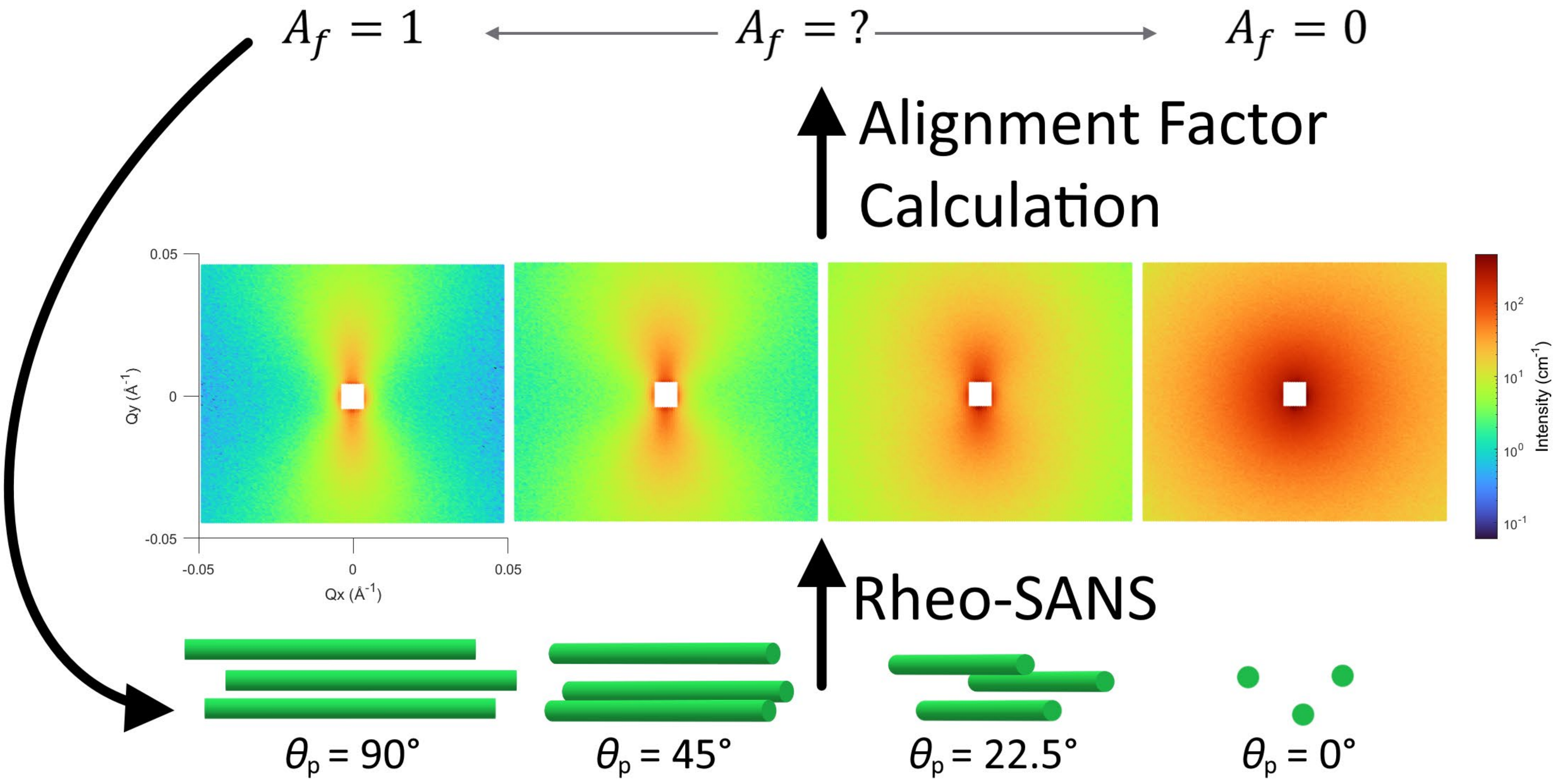

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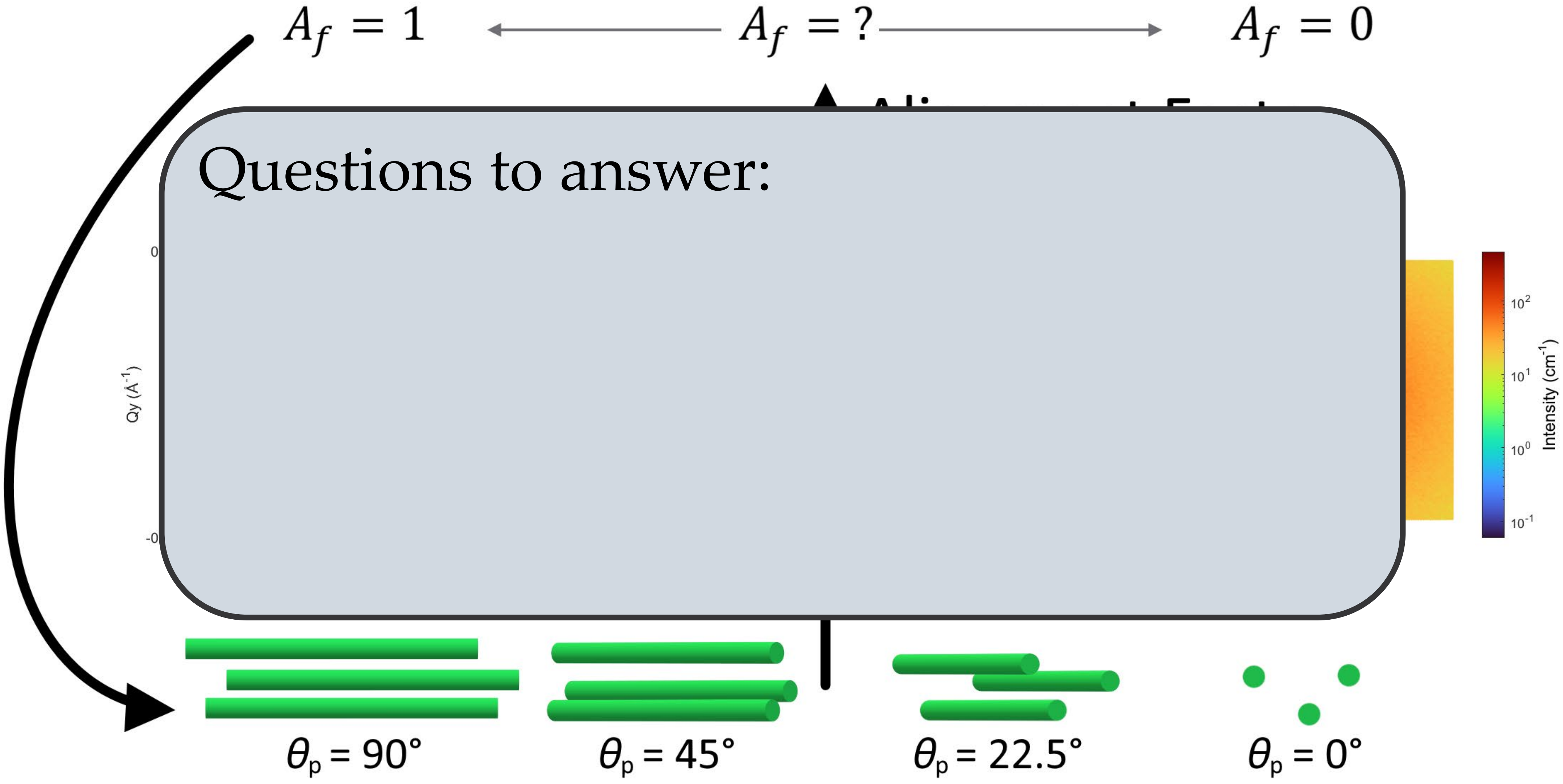
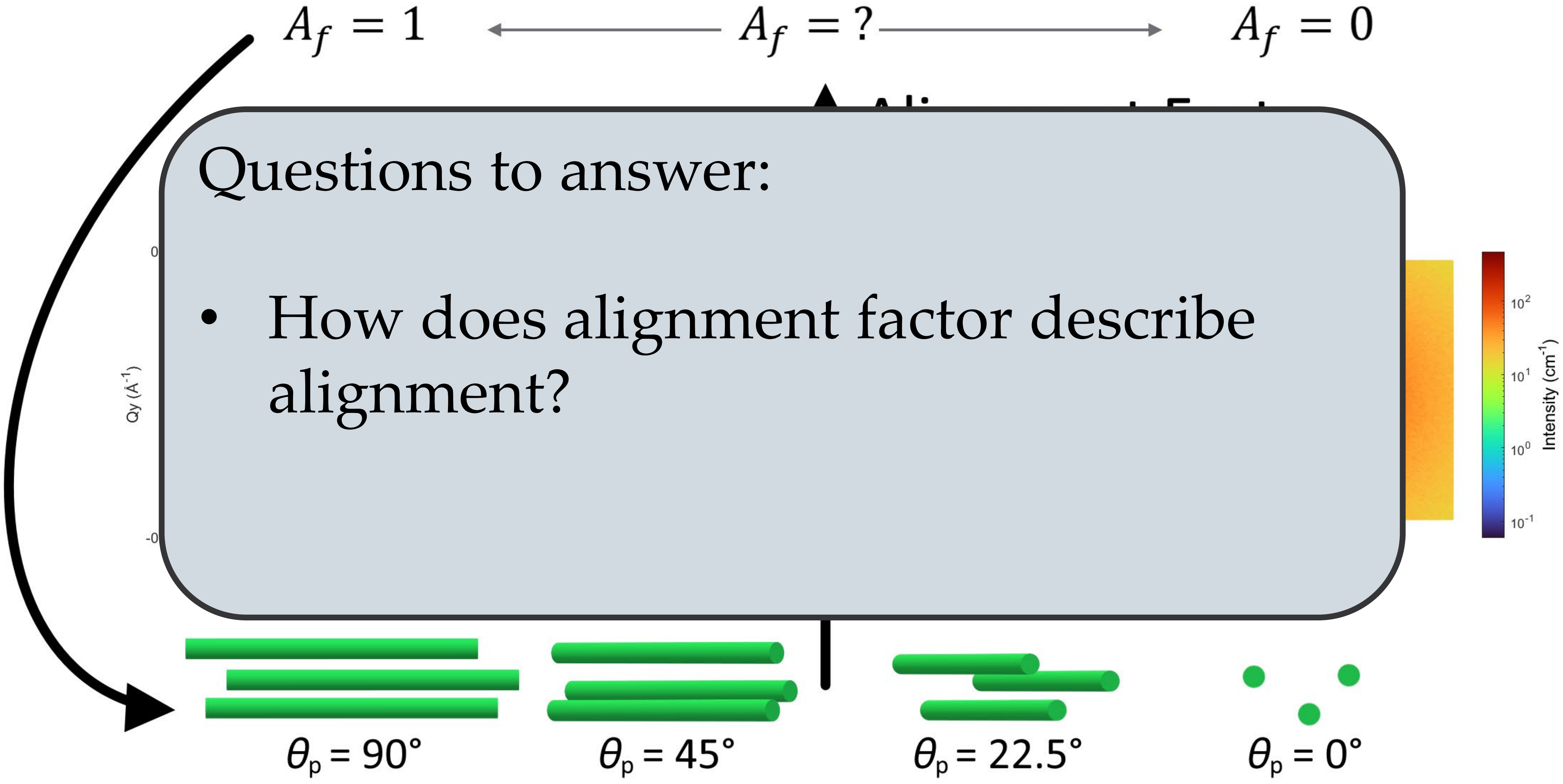


Questions to answer:

Characterizing Alignment



Questions to answer:

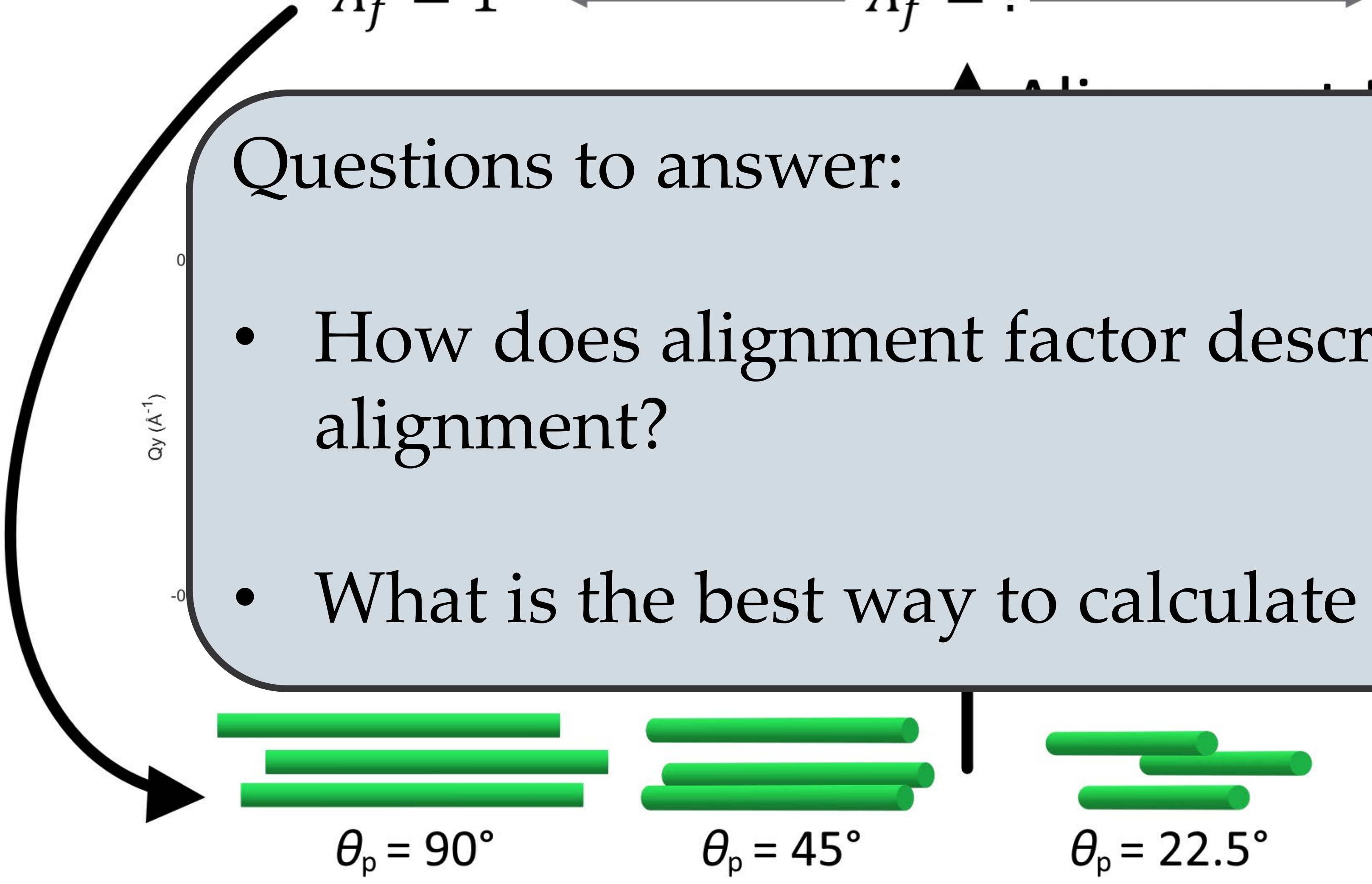
- How does alignment factor describe alignment?

Characterizing Alignment

$A_f = 1$ ⟵ $A_f = ?$ ⟶ $A_f = 0$

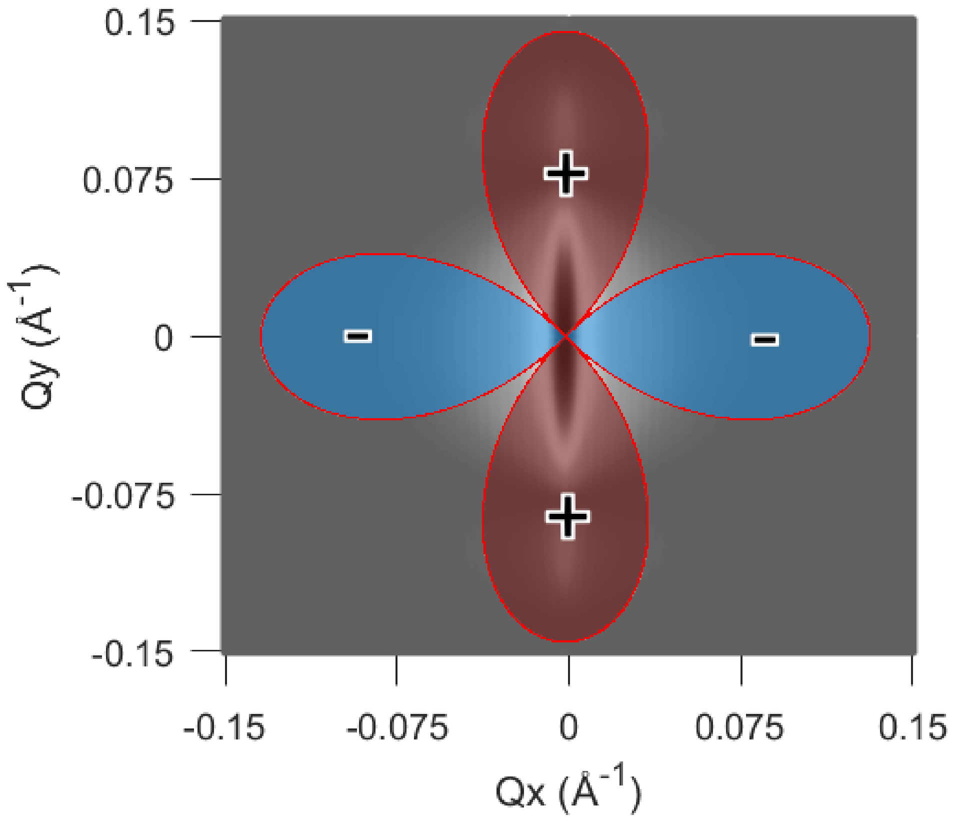
Questions to answer:

- How does alignment factor describe alignment?
- What is the best way to calculate it?



Differences in Calculation Methods

Cosine expansion



Differences in Calculation Methods

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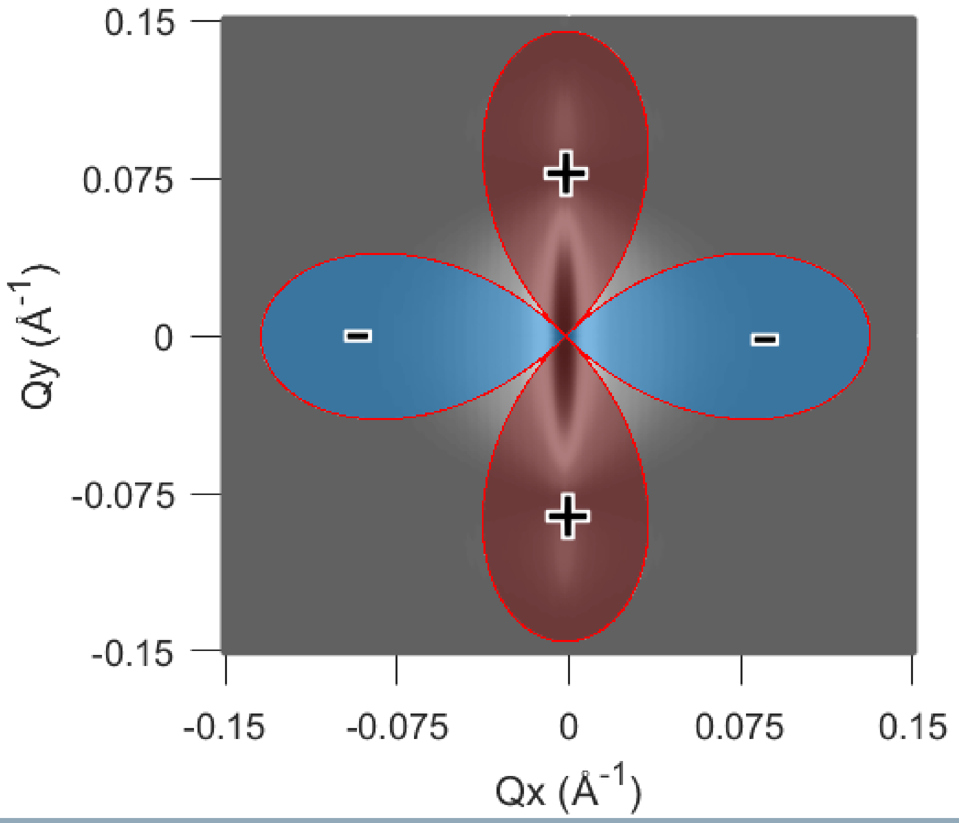
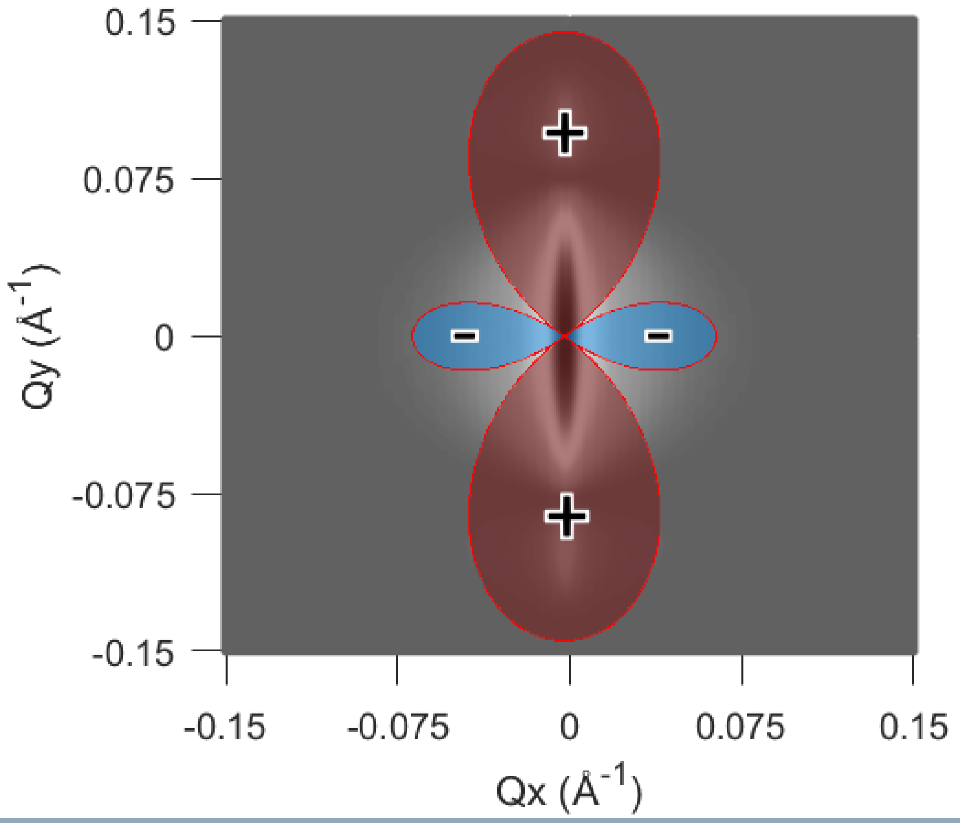


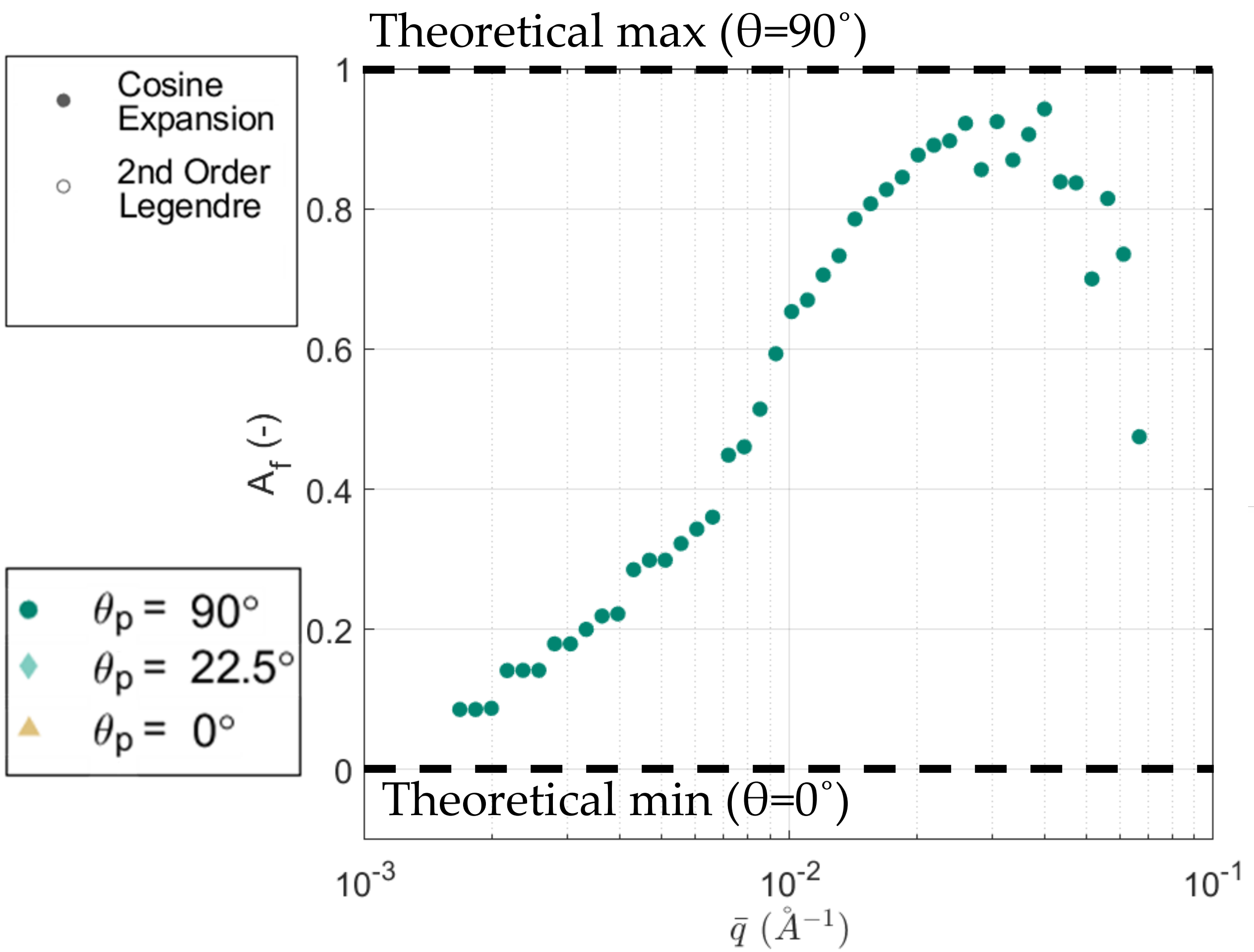
Walker, et. al., Macromolecules **29** (1996)
https://doi.org/10.1021/ma951127p

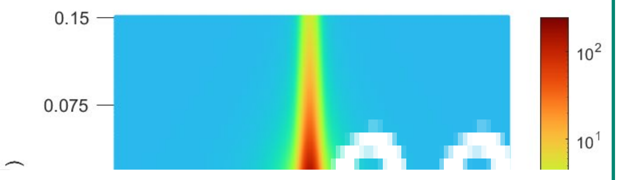
2nd order Legendre



Hayward, et. al., Rev. Sci. Instrum. **92** (2021)
https://doi.org/10.1063/5.0040675

Alignment Factor From Series Expansion





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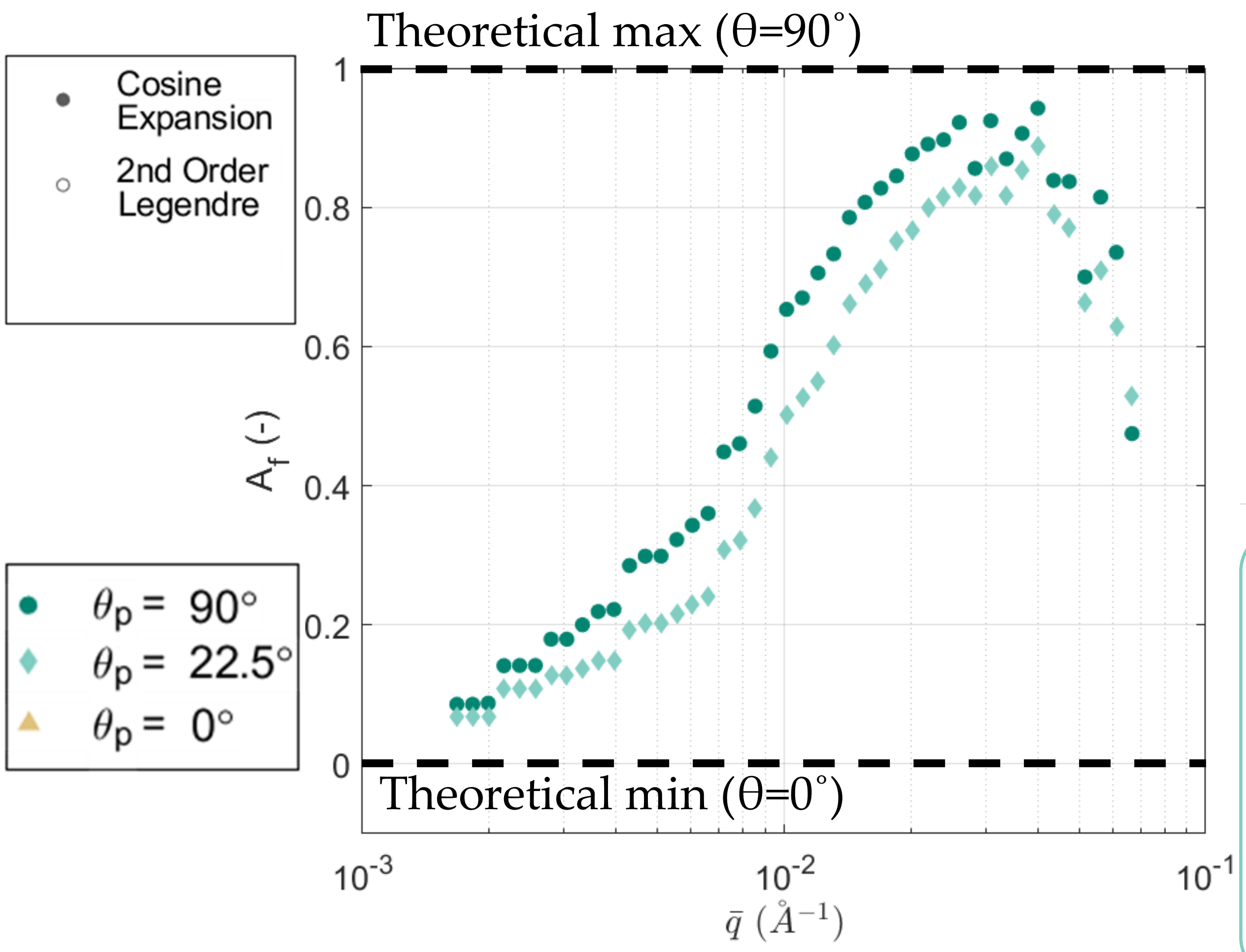

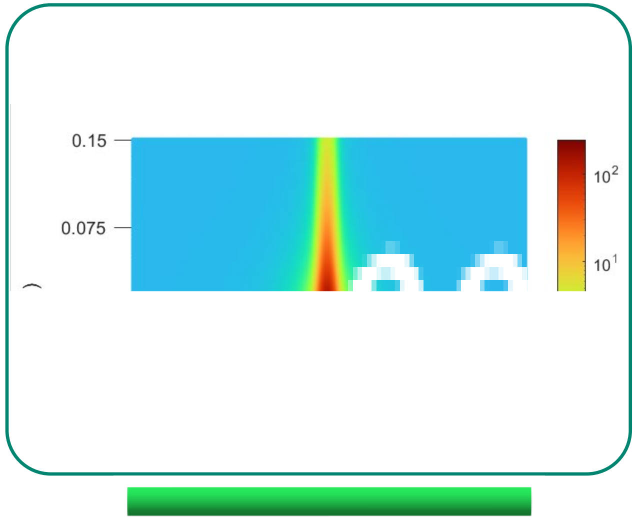

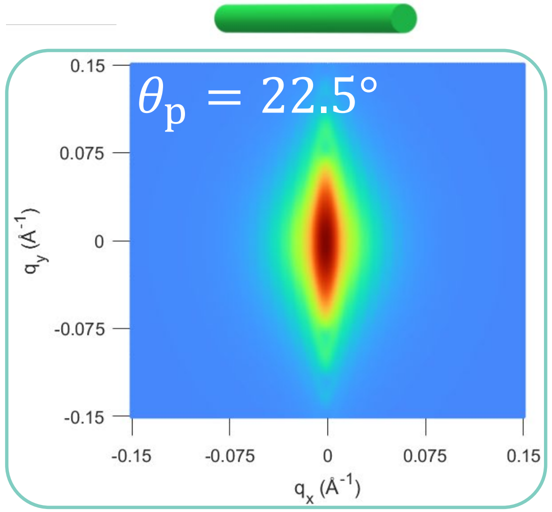

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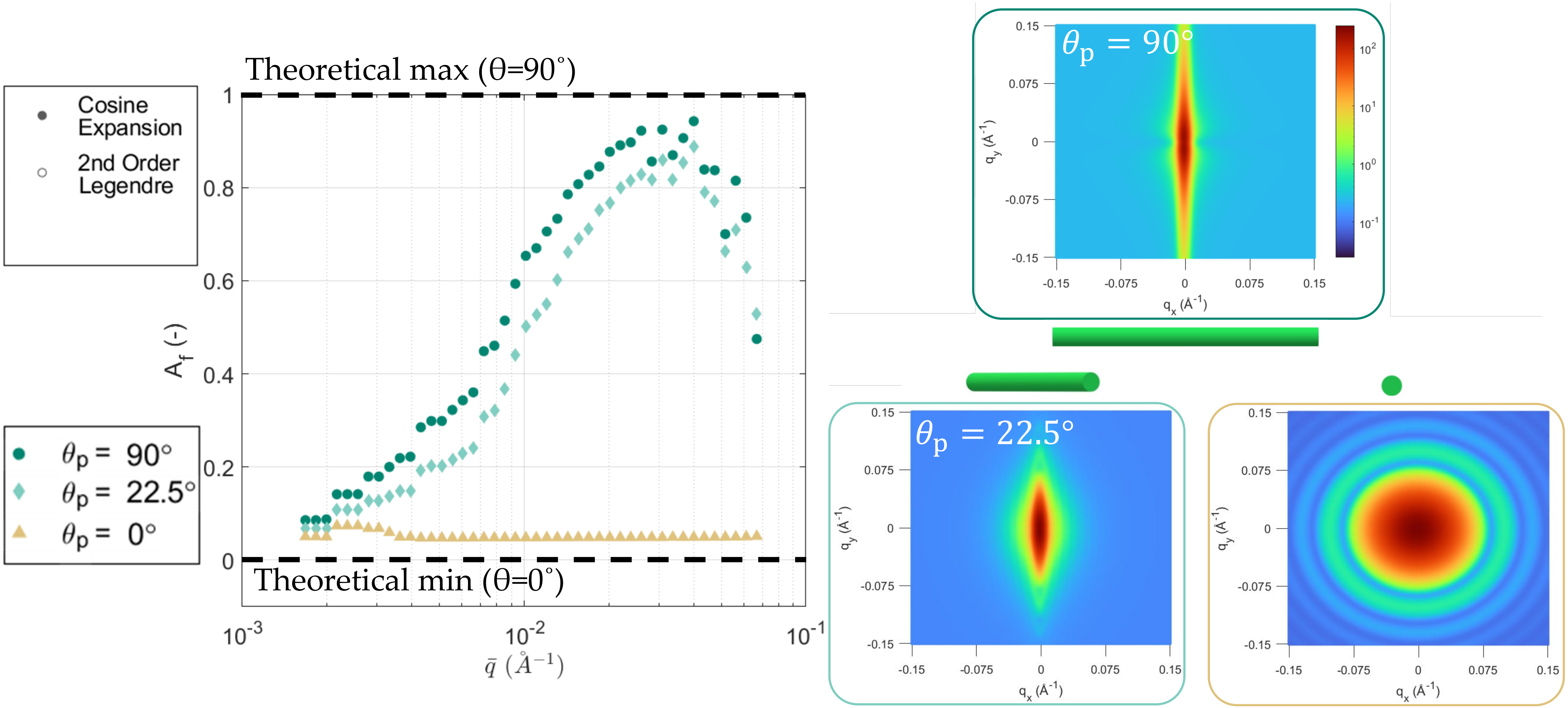

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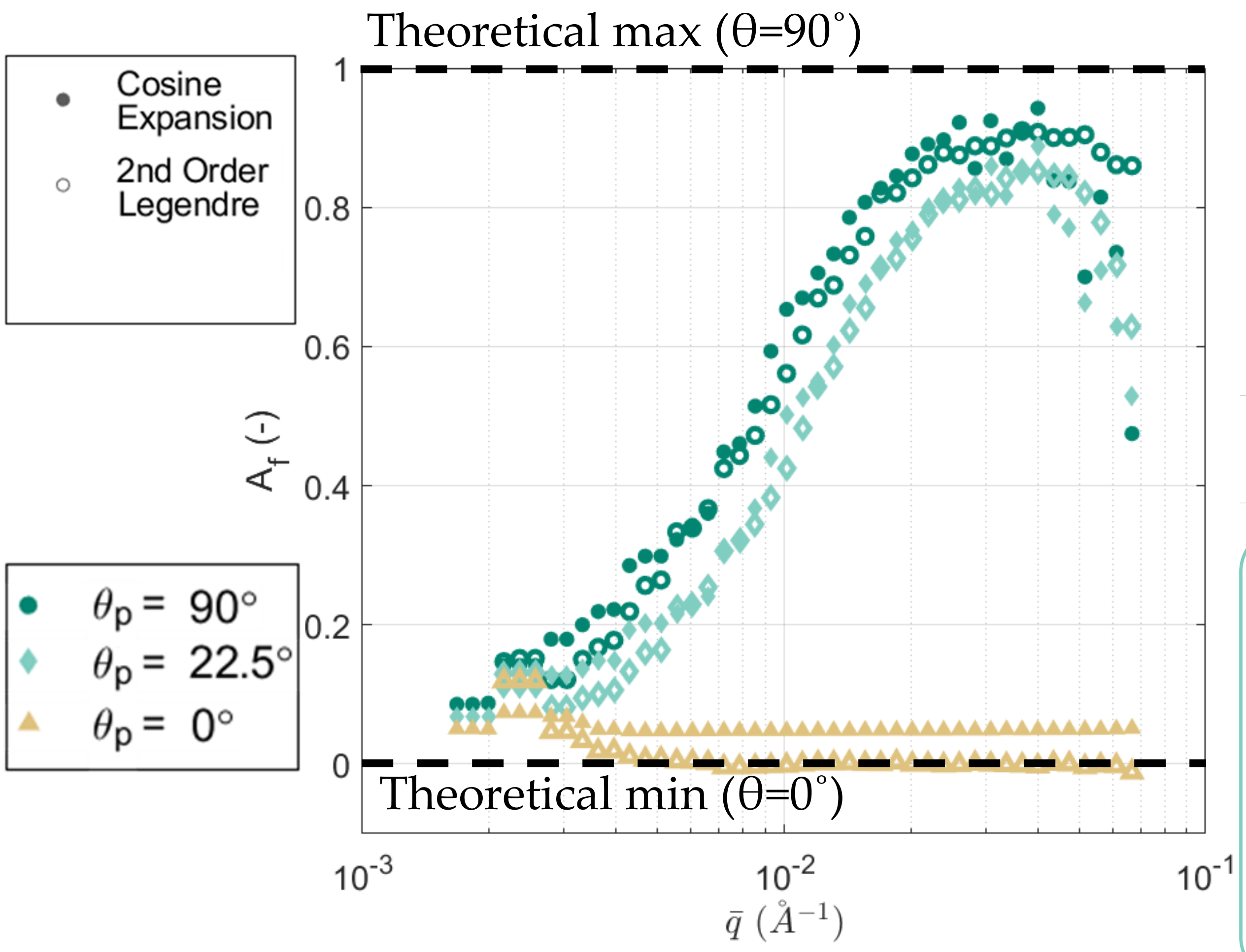
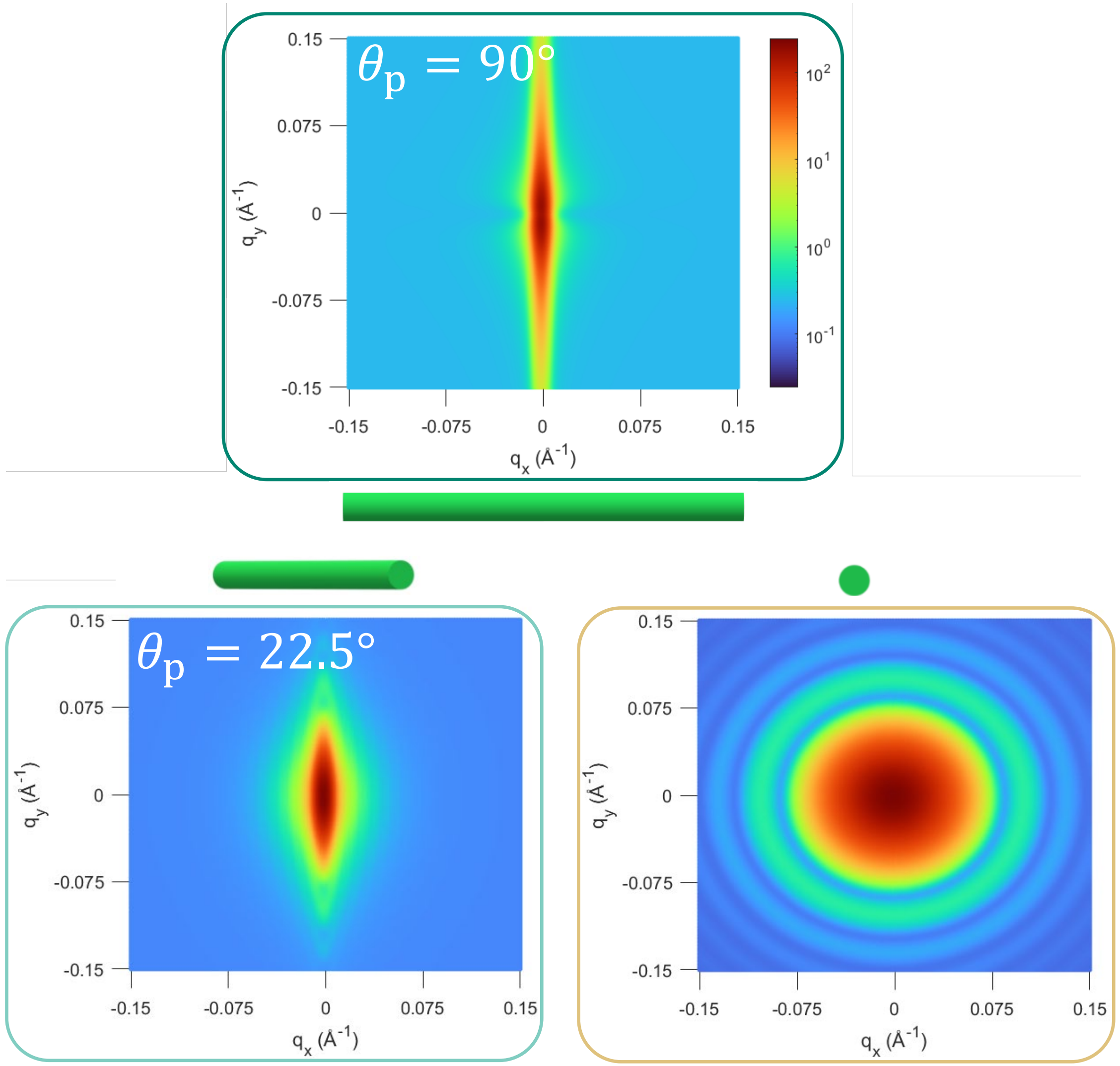
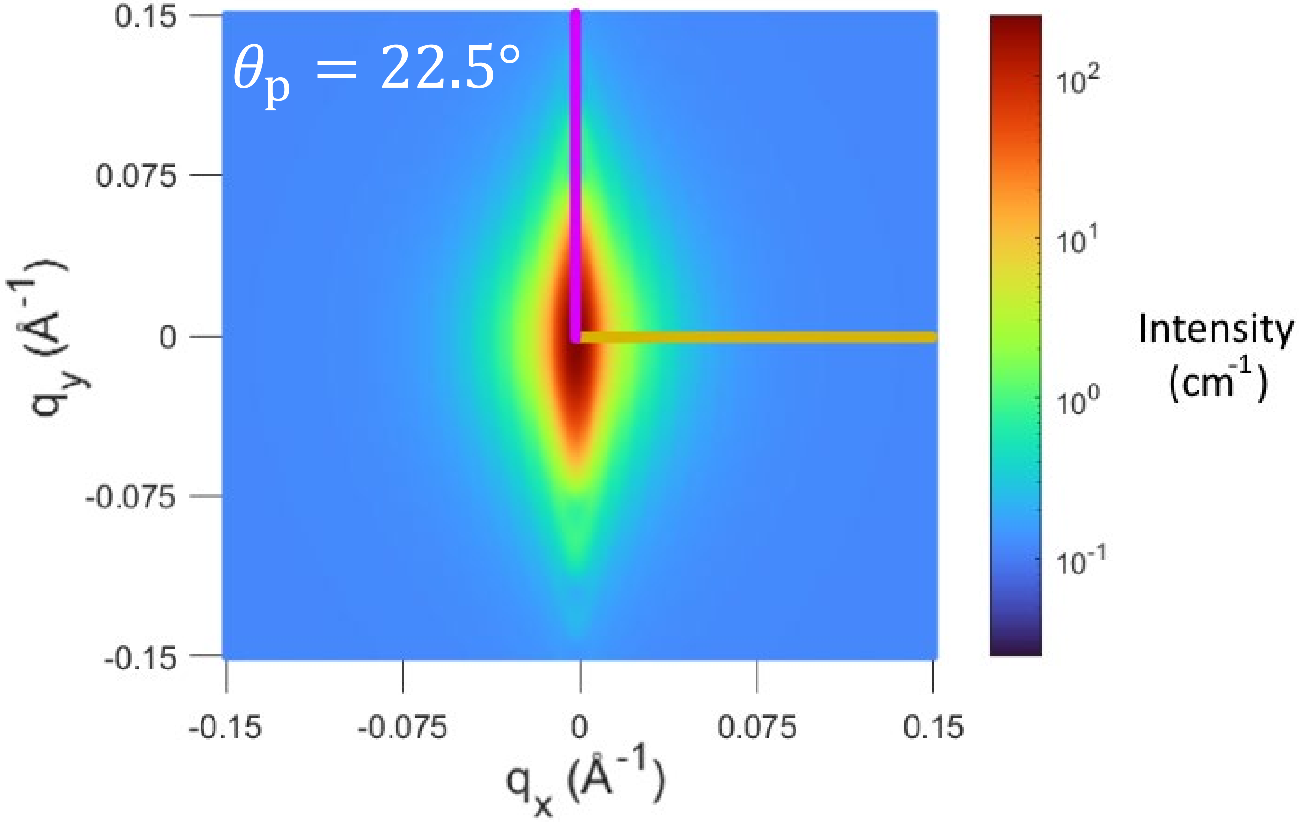




Calculating Alignment Factor – Integrated Axes



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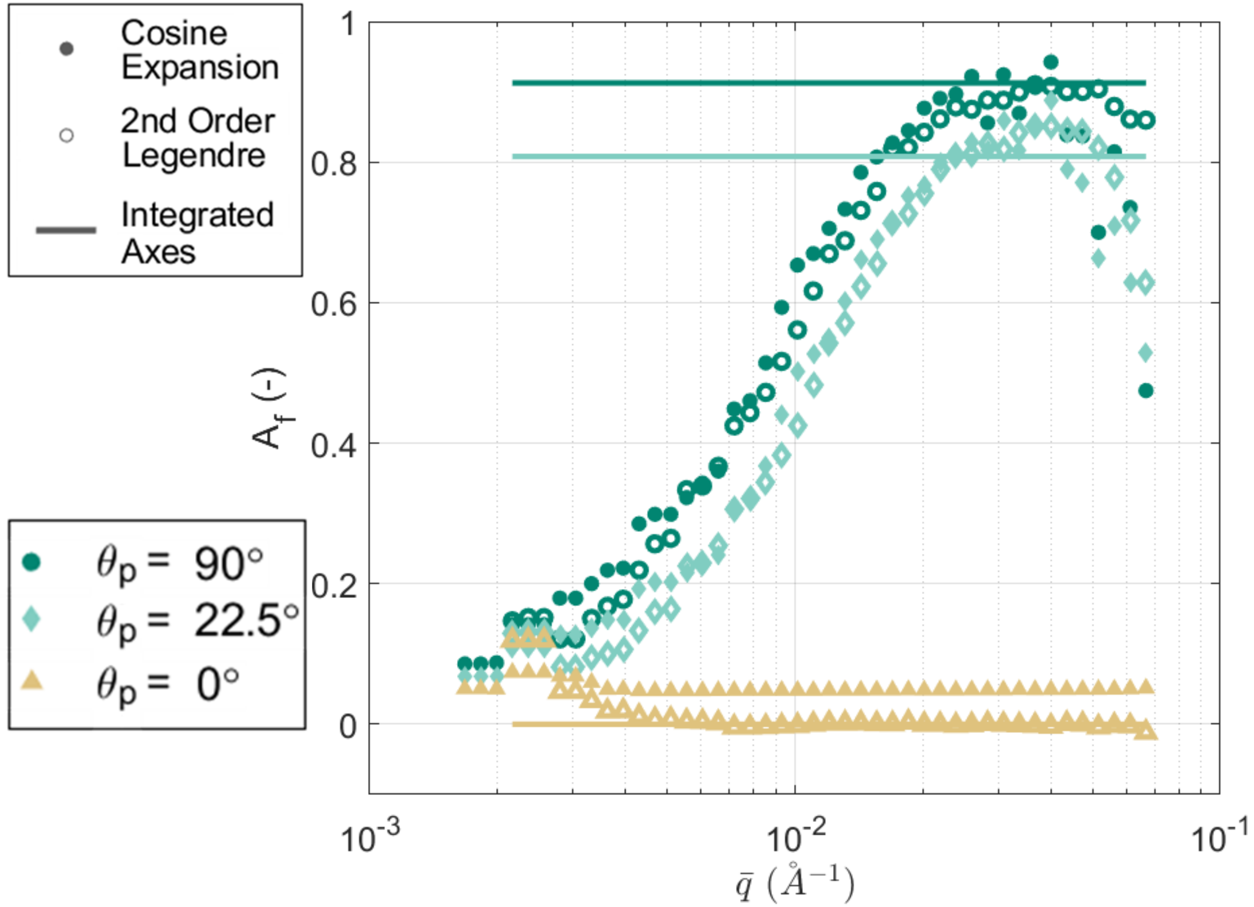
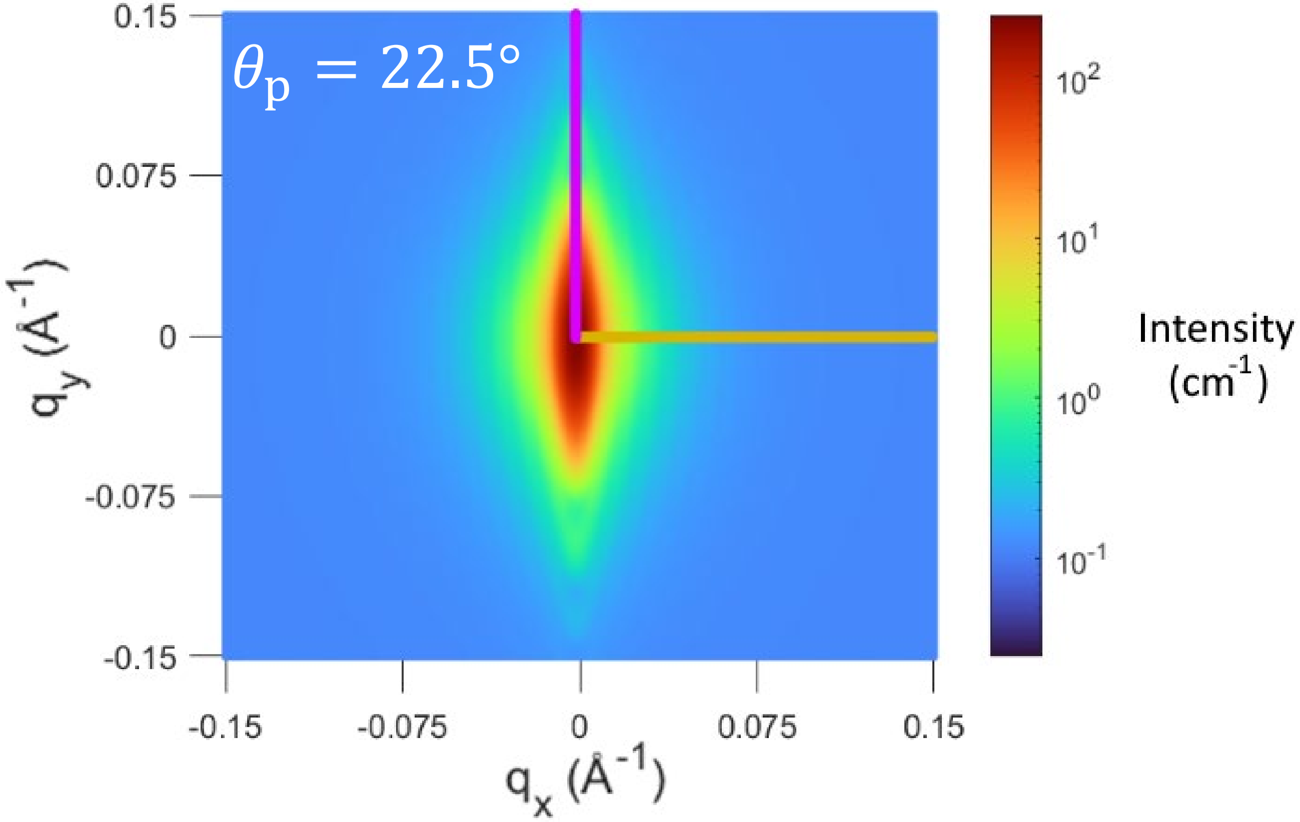
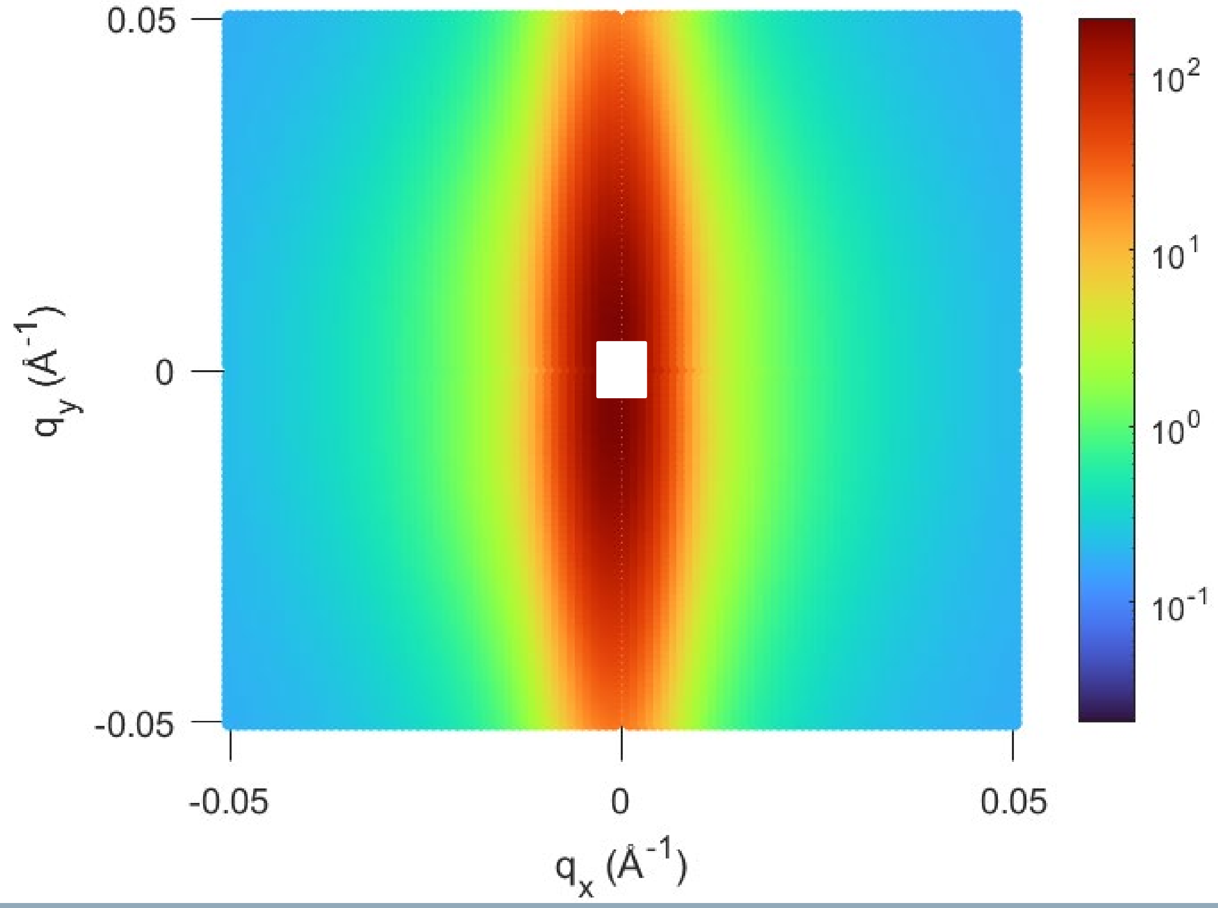


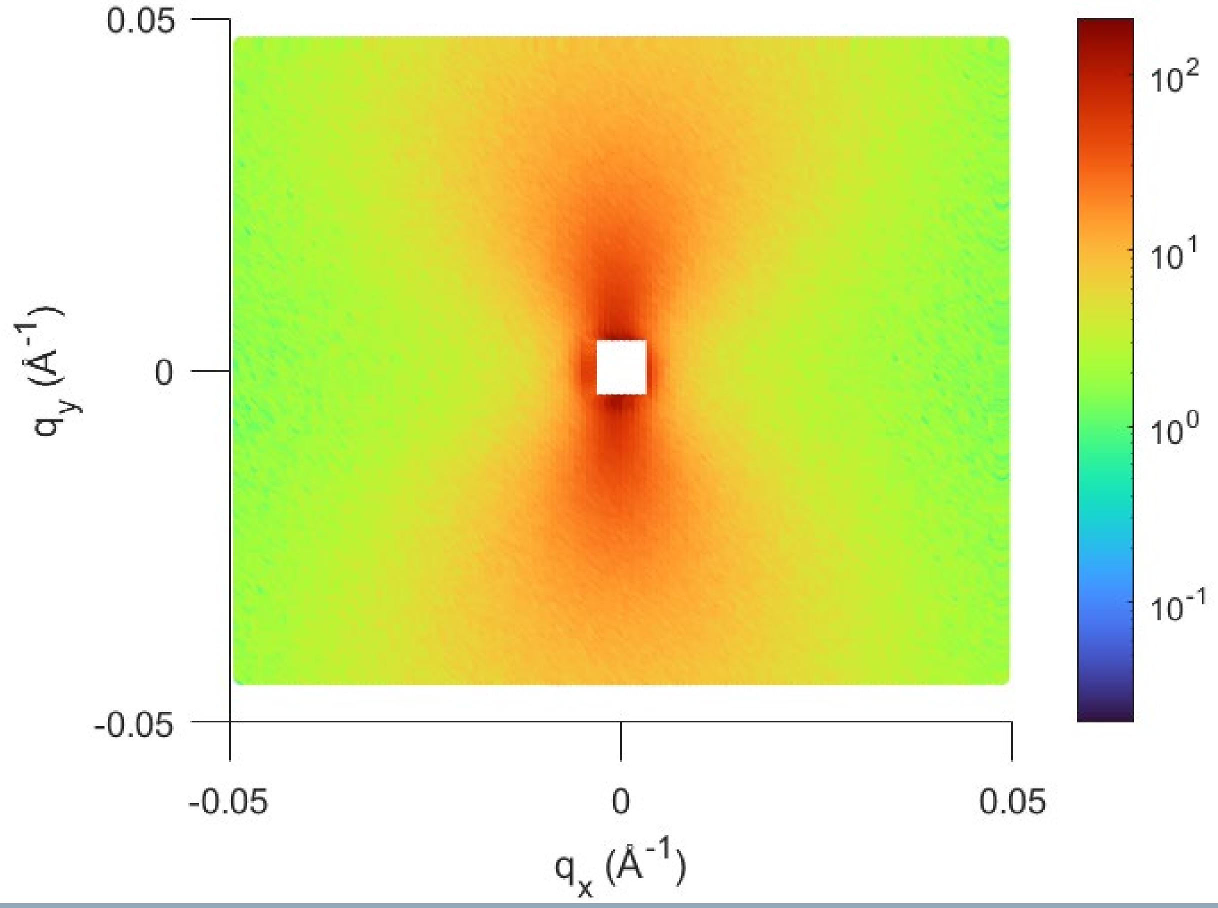


Reminder: Scattering Pattern Shapes

Theoretical

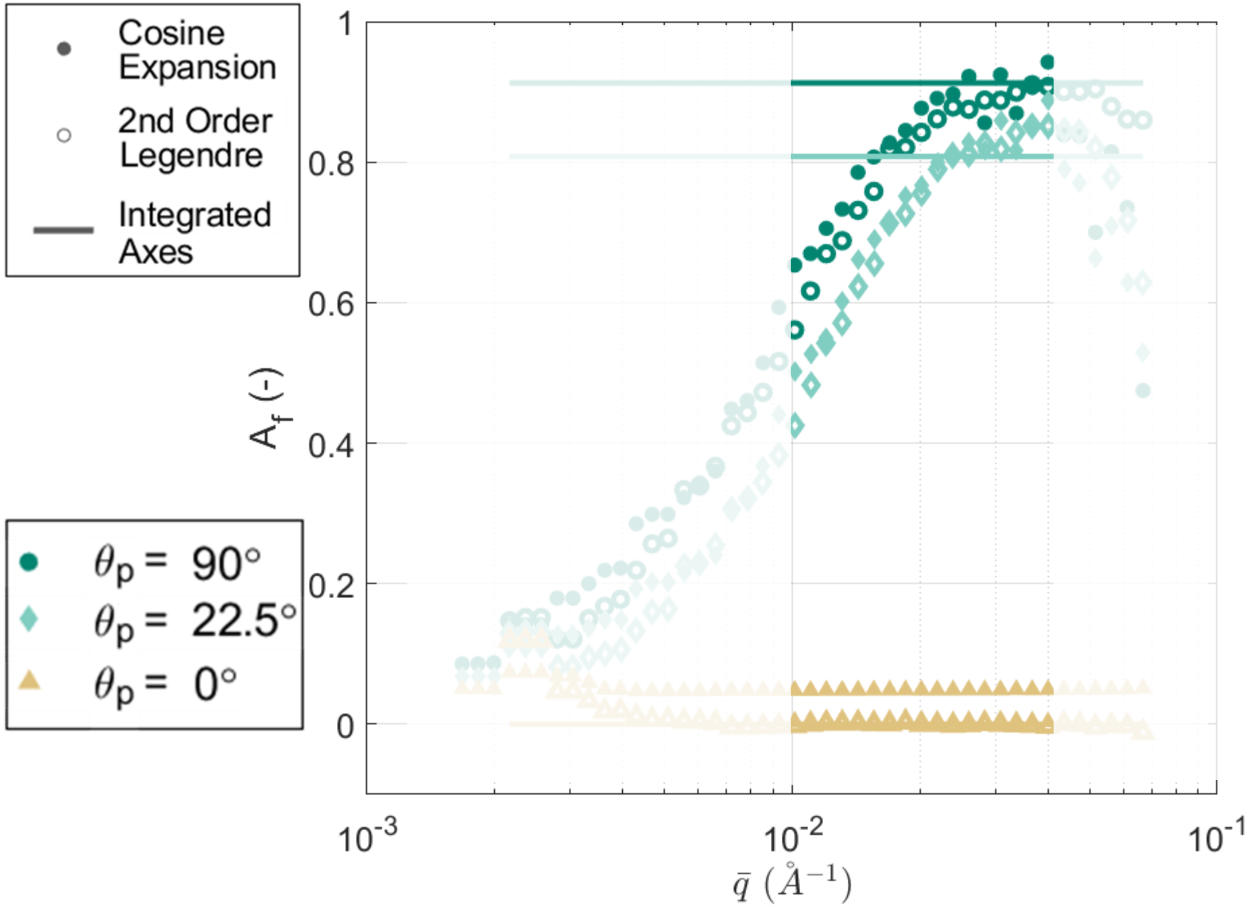


Experimental

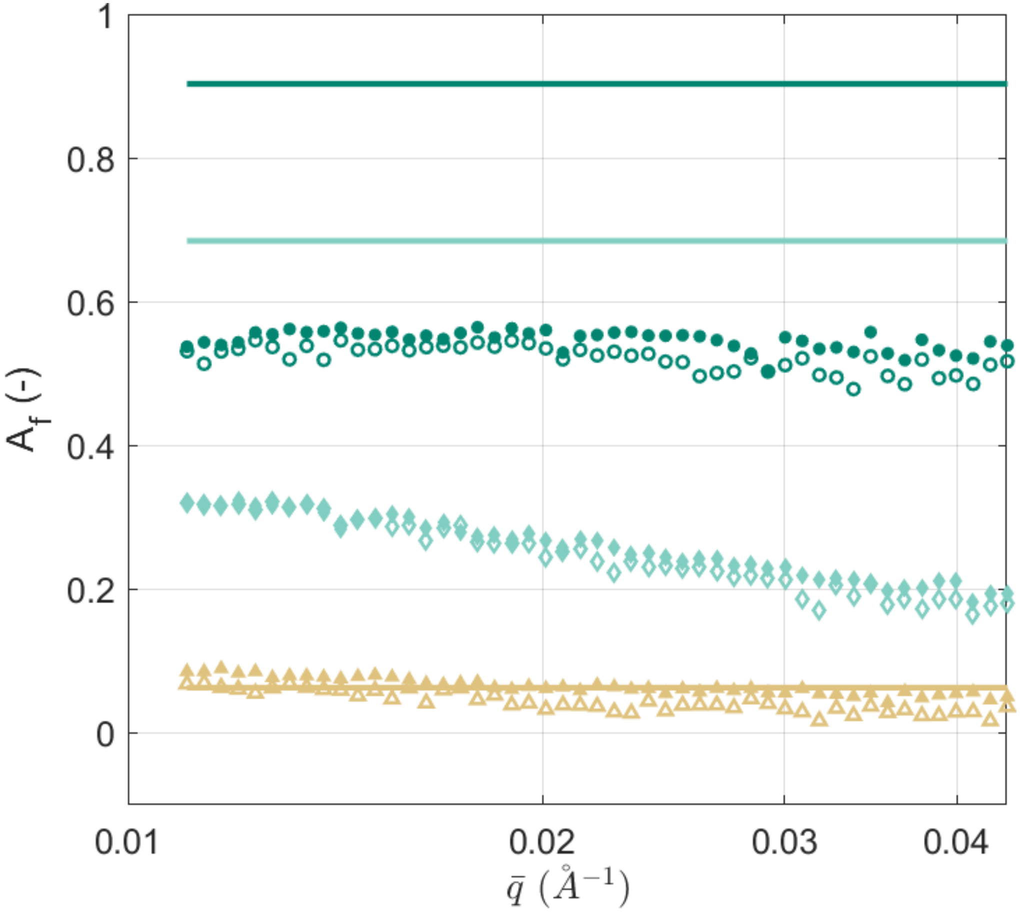


Comparison

Theoretical

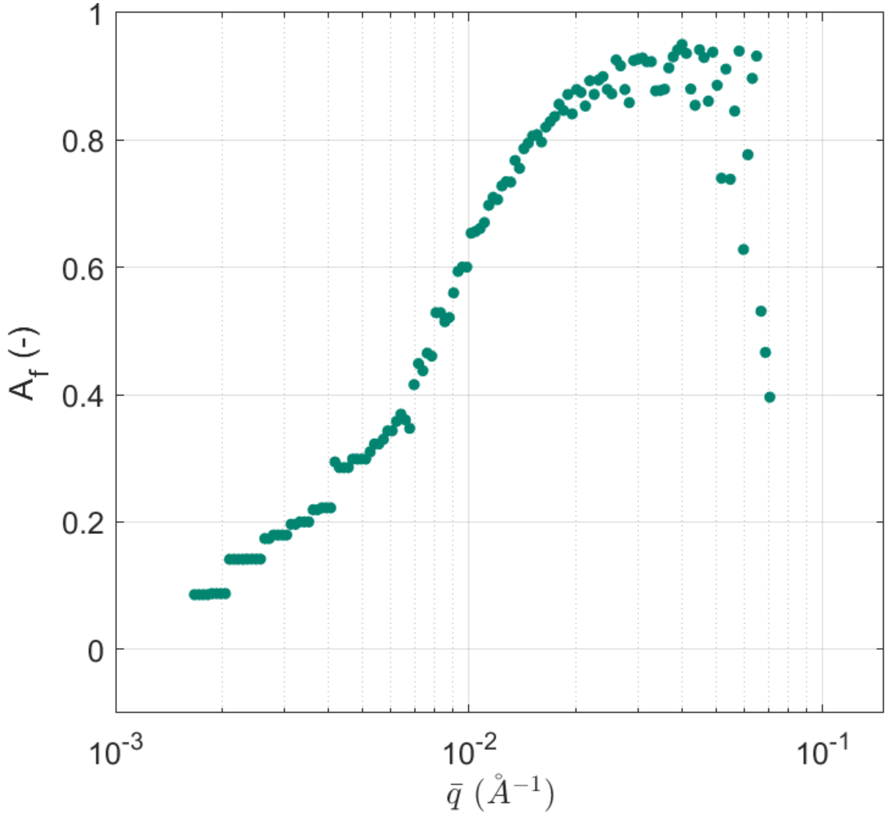


Experimental

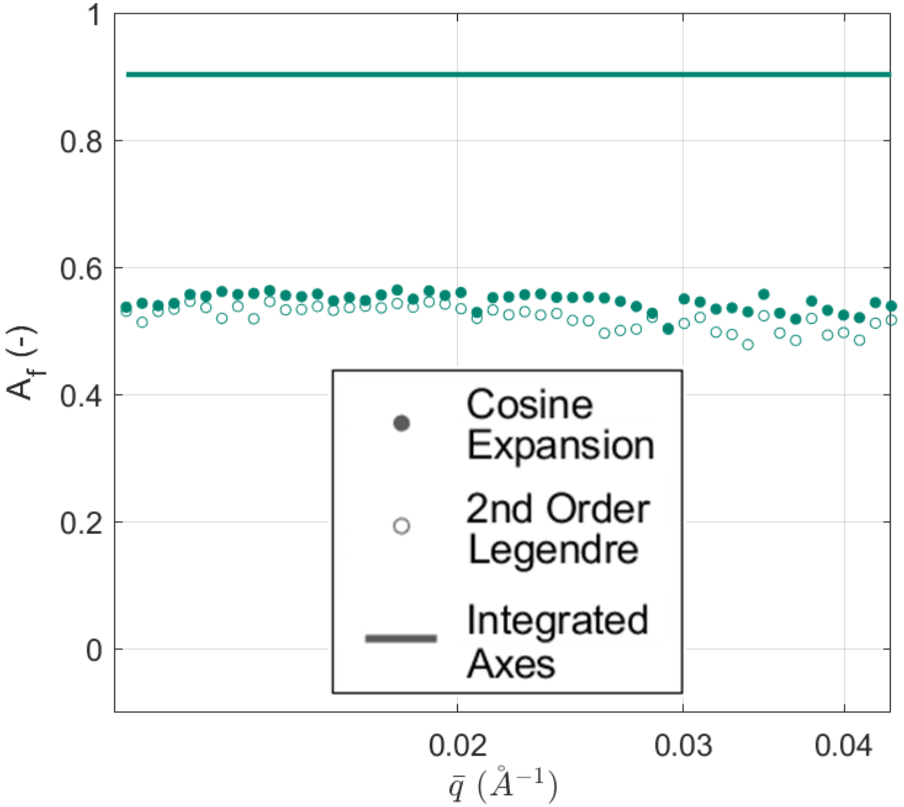


Summary

Location matters



Methods not equivalent



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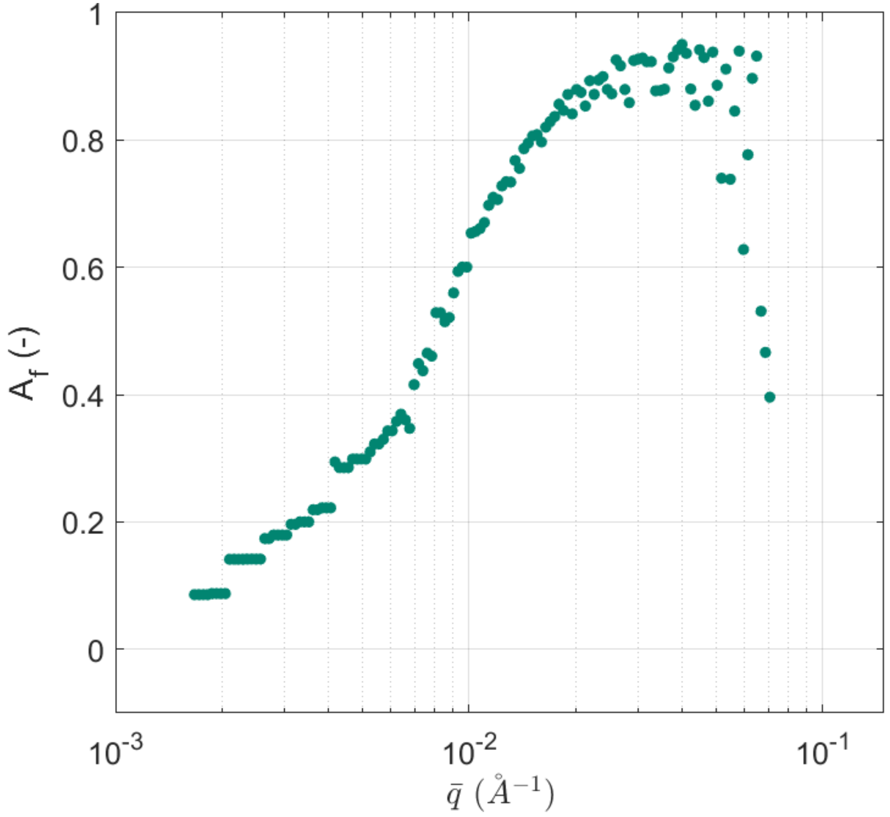

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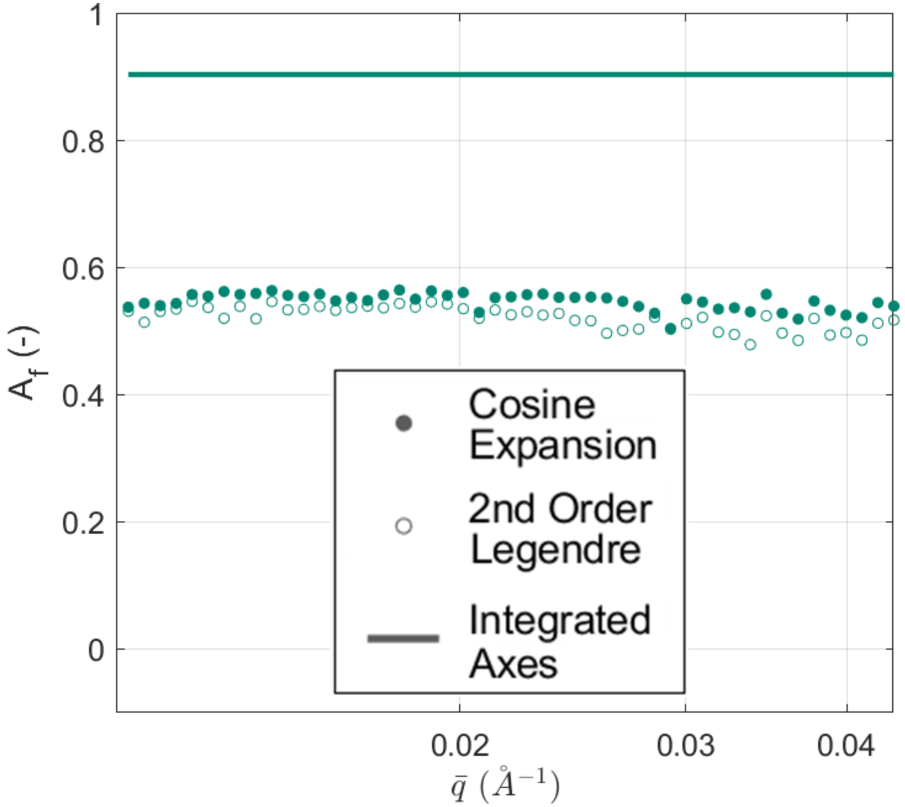
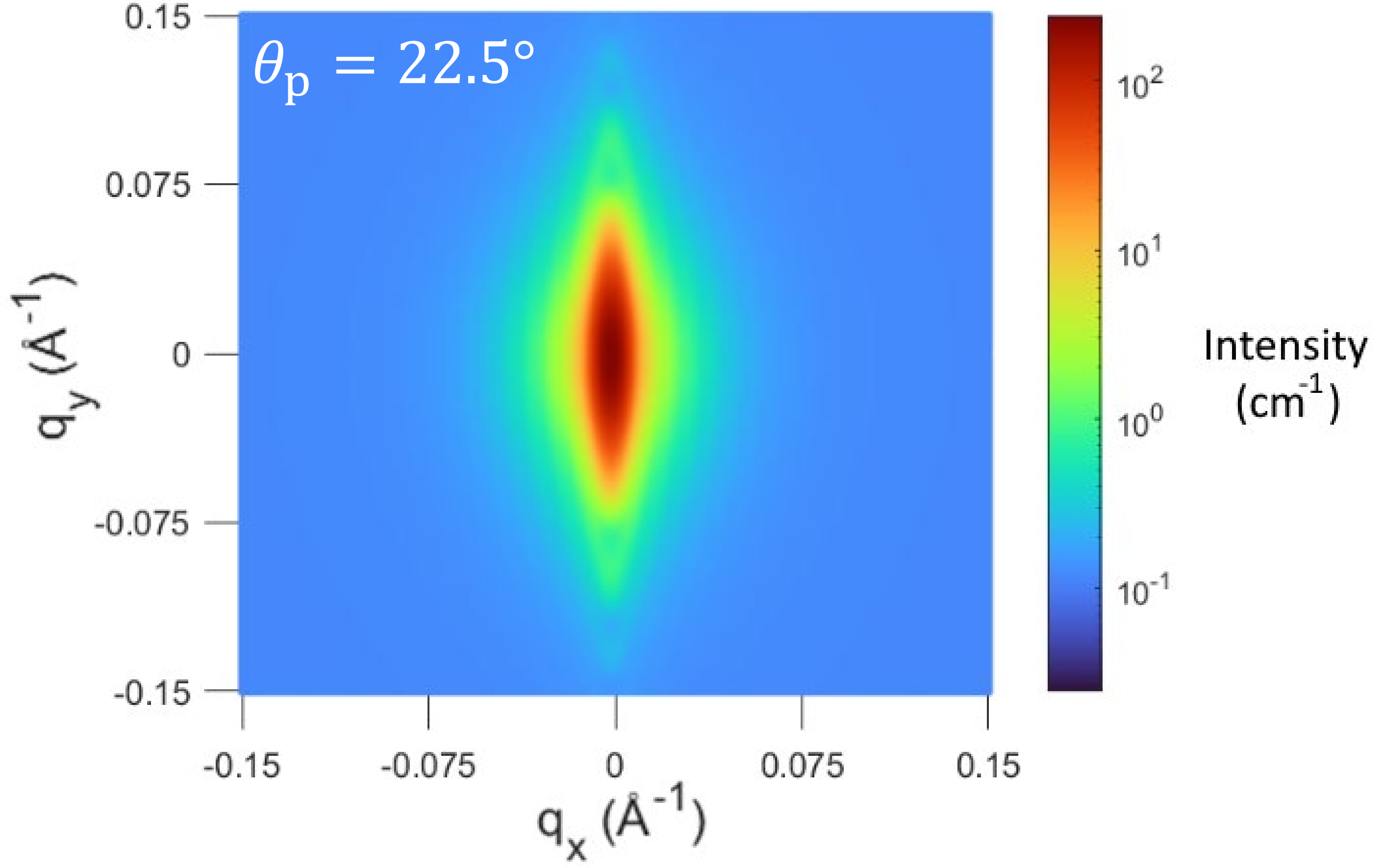


Future Plans

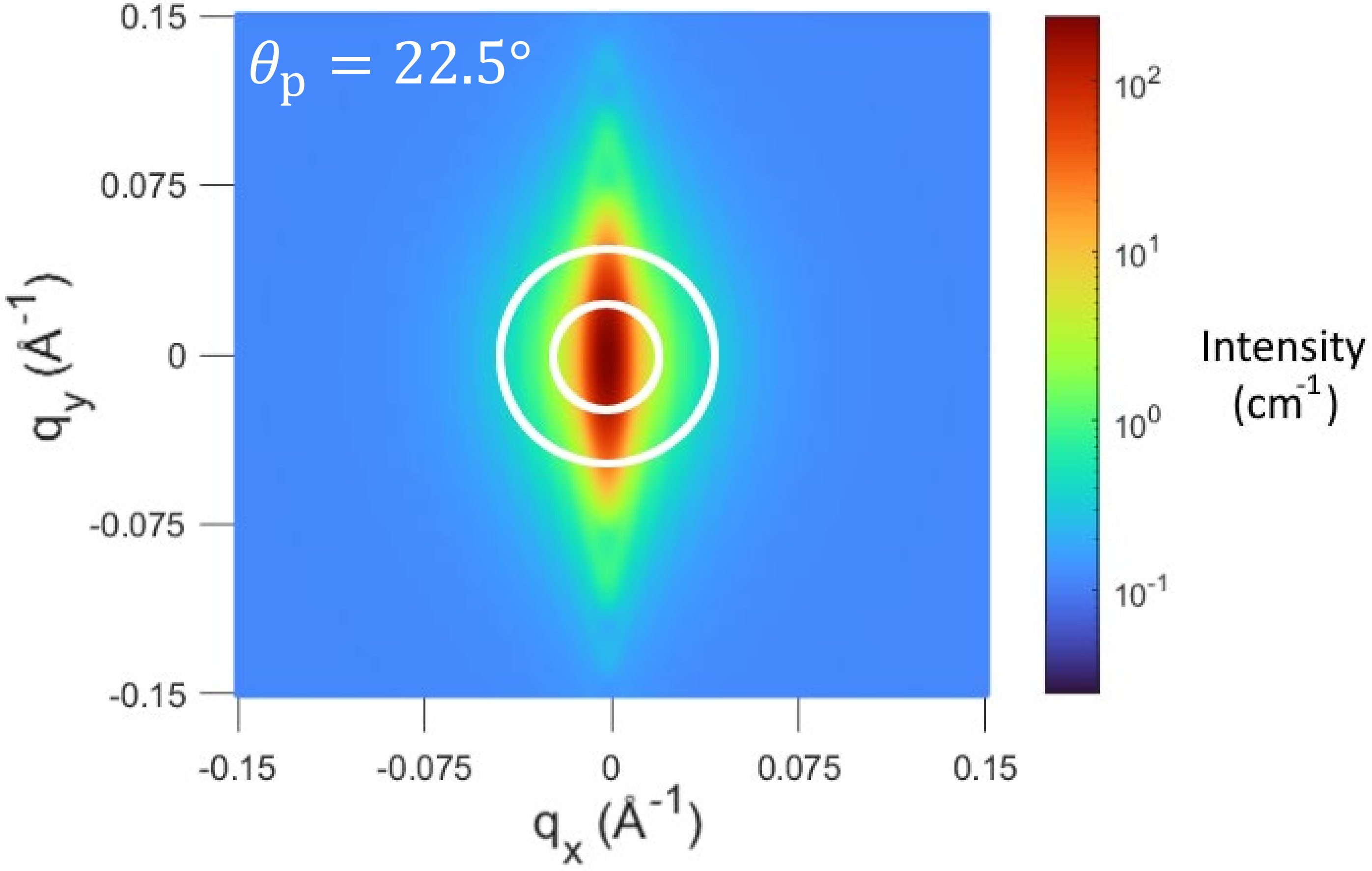
- Determine particle orientation between radial and tangential configurations
- Which alignment factor describes particle orientation best?

Supplementary slides

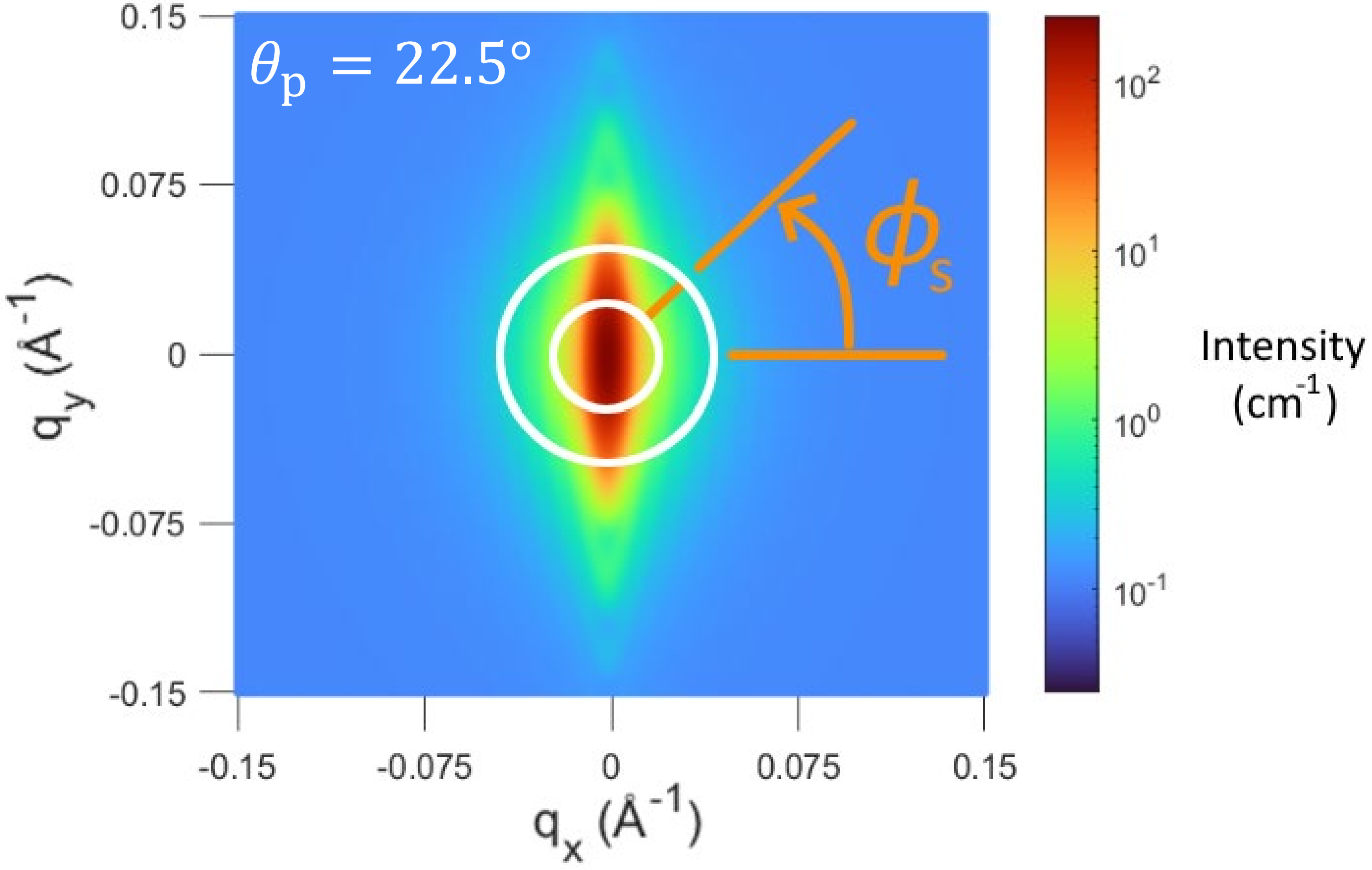
Cosine expansion and Legendre polynomial



Cosine expansion and Legendre polynomial



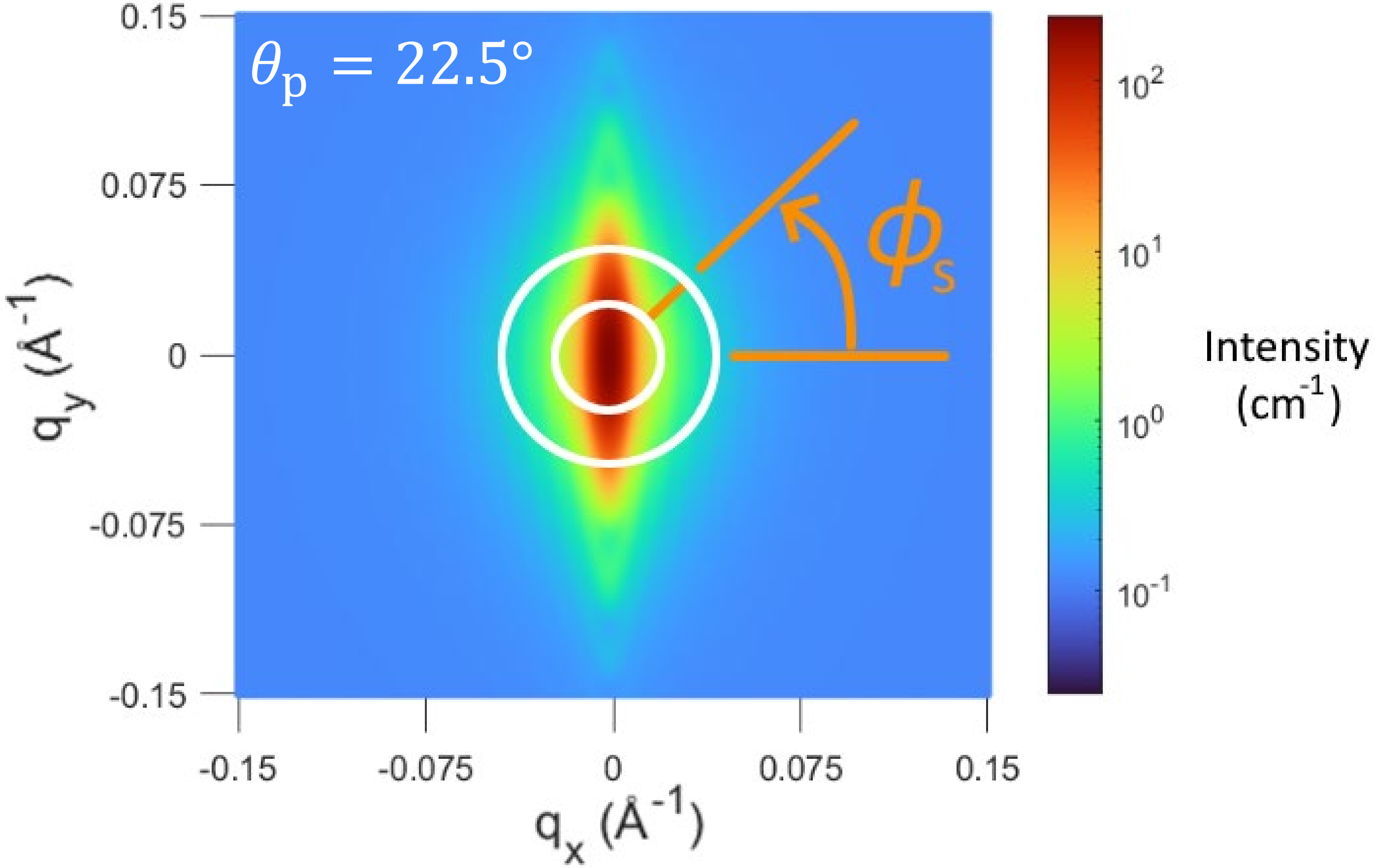
Calculating Alignment Factor – Series Expansion



Calculating Alignment Factor – Series Expansion

Cosine expansion

$$A_f(q) = \frac{\int_0^{2\pi} I(q,\phi_s)\cos 2(\phi_s - \phi_{s,0})\, d\phi_s}{\int_0^{2\pi} I(q,\phi_s) d\phi_s}$$



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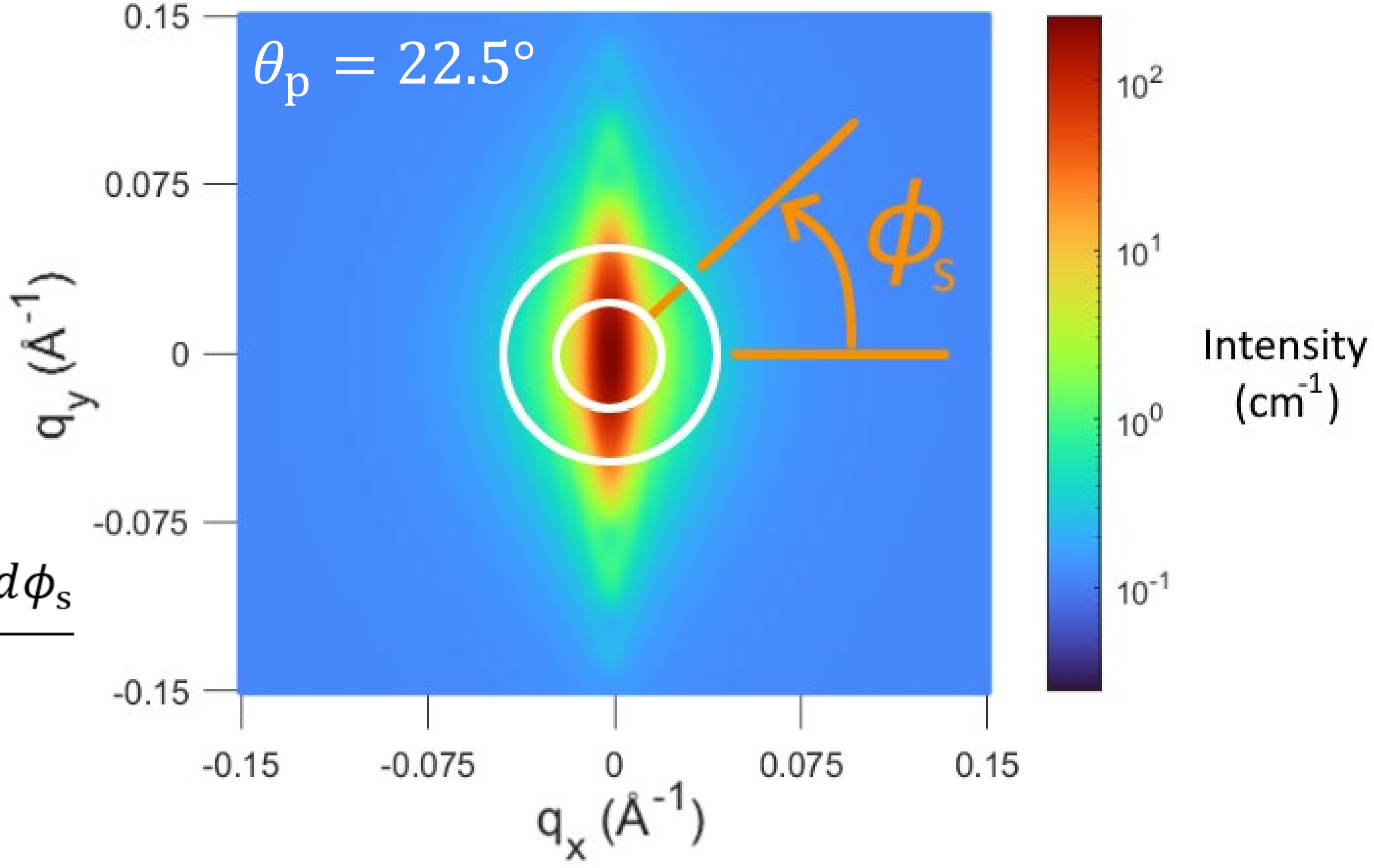
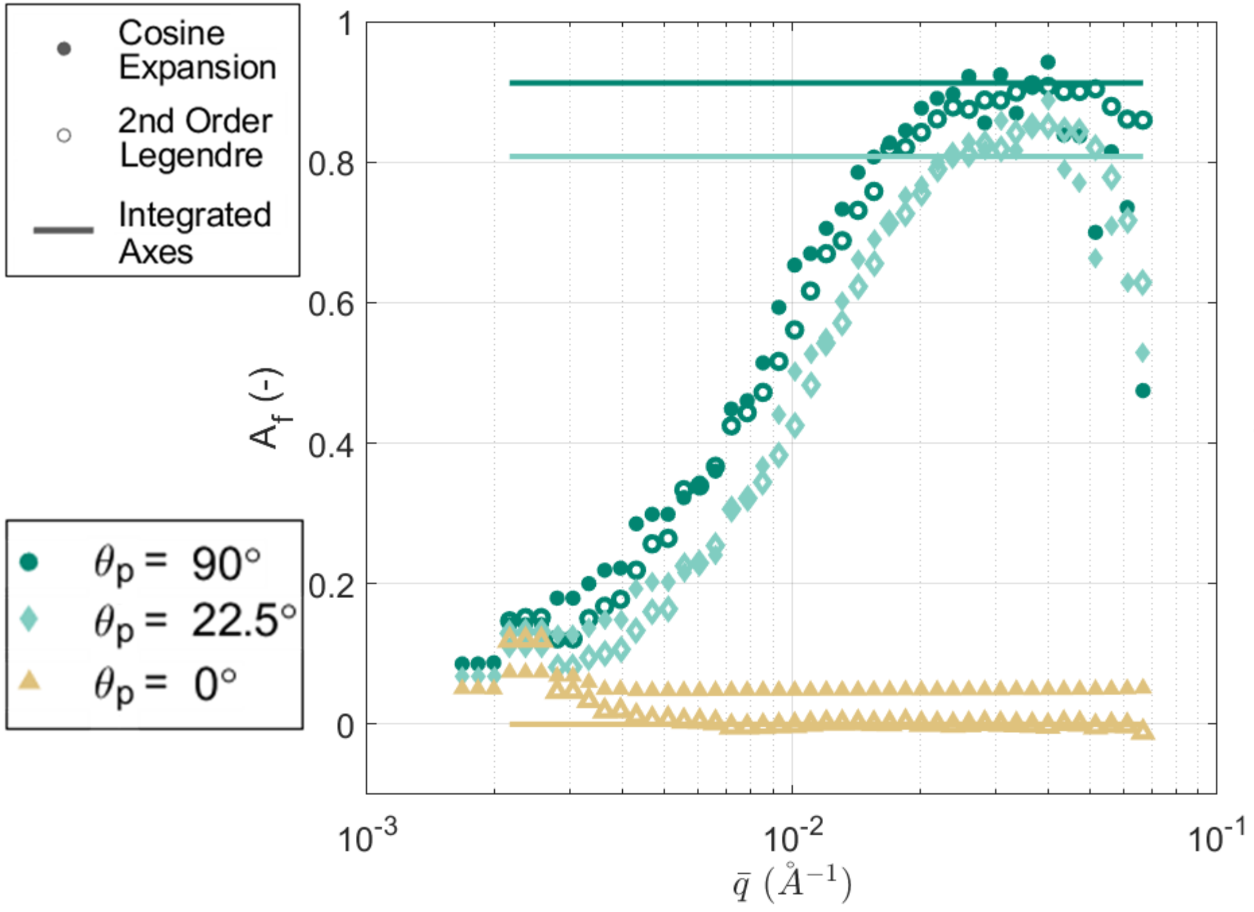
2nd order Legendre

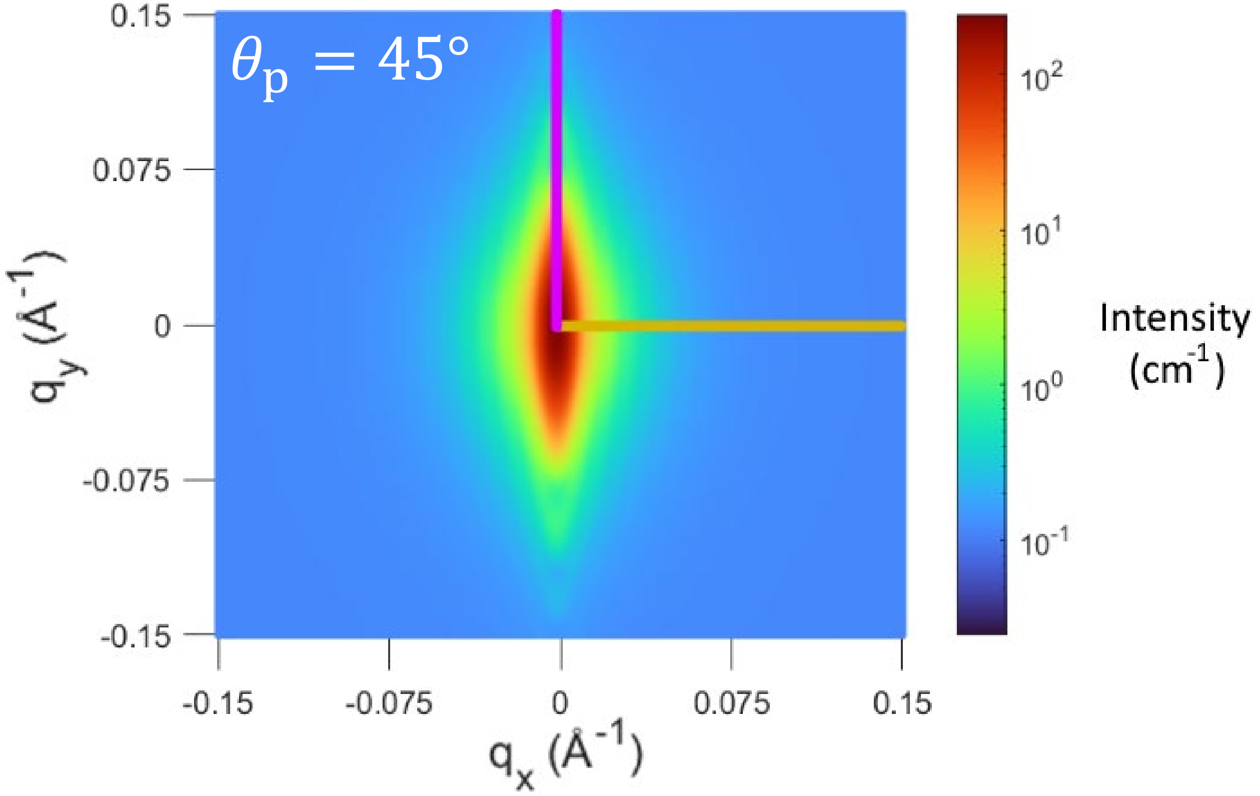
$$A_f(q) = -2\frac{\int_0^{\pi} I(q,\phi_s)\left(\frac{3}{2}\cos^2\phi_s - \frac{1}{2}\right)\sin\phi_s\,d\phi_s}{\int_0^{\pi} I(q,\phi_s)\sin\phi_s\,d\phi_s}$$



Calculating Alignment Factor – Integrated Axes



$$A_f = \frac{\int_{q_{min}}^{q_{max}} I_\perp(q)\,dq - \int_{q_{min}}^{q_{max}} I_\parallel(q)\,dq}{\int_{q_{min}}^{q_{max}} I_\perp(q)\,dq}$$



Calculating Alignment Factor – Integrated Axes