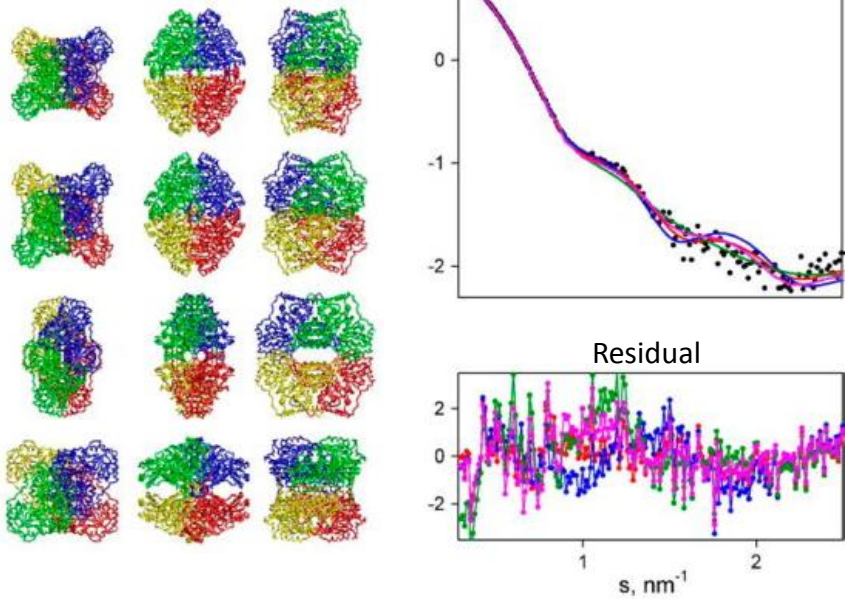
SANS Inversion Via Magnetic Tagging

Kathryn Krycka, Erik Brok, Chuck Majkrzak

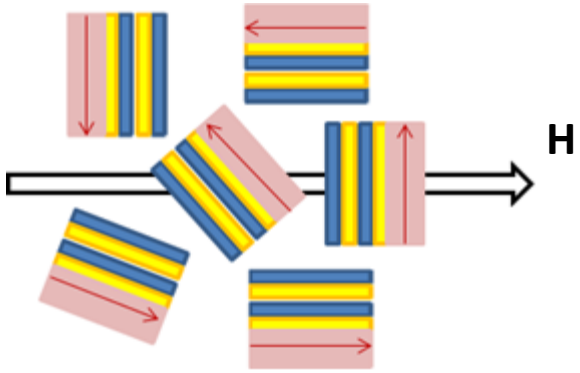
Fixed-Tag, Phase Recovery: "Killing two birds with one stone"

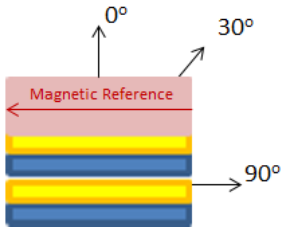
(A) Obtain unique scattering amplitude (magnitude + phase), rather than potentially non-unique scattering intensity (magnitude squared)

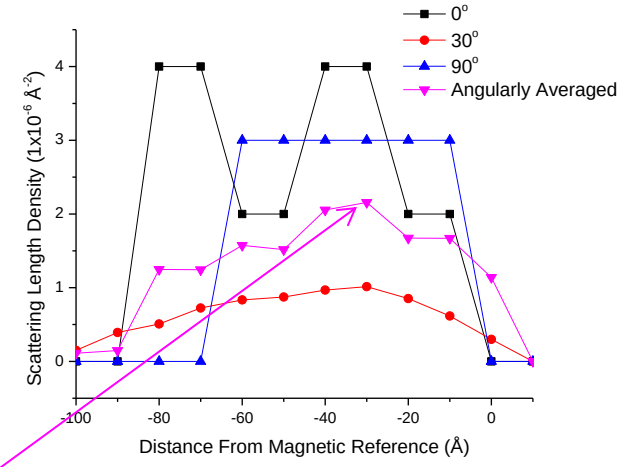


M.V. Petoukhov and D.I. Svergun, Biophysical Journal, **89,** 1237–1250 (2005).

(B) Reference *fixed* relative to sample additionally removed the SANS Rotational Averaging (shown in *2D*)

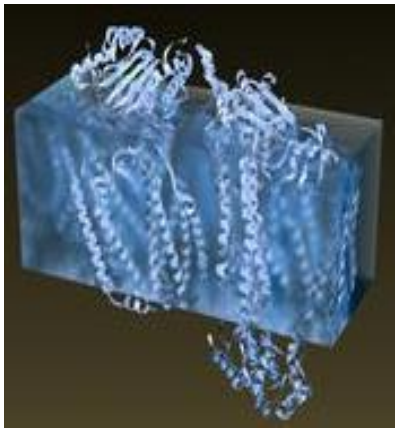






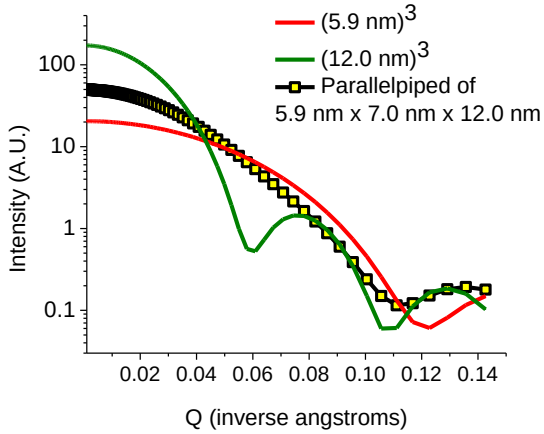
Conventional SANS

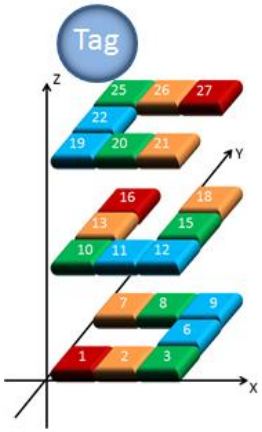
Eventual Goal (3D Inversion)

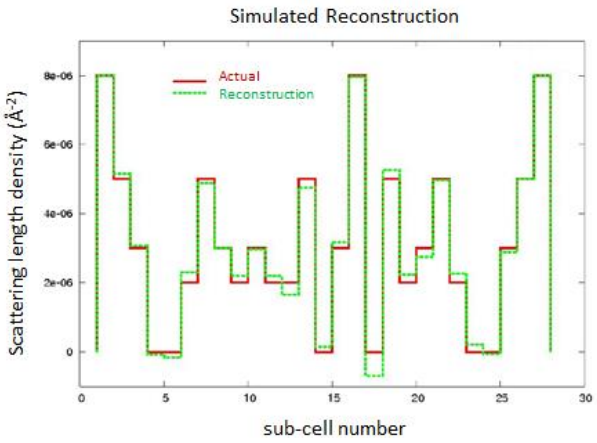


K. A. Rubinson, C. Pokalsky, S. Kruegar, L. J. Prochaska, *Protein J.*, 32, 27-38, 2013

- Quantifying complex *3D* structures with non-uniform dimensions is challenging in conventional SANS
- C. oxidase in which parameters of 5.9nm x 7.0nm x 12.0nm were carefully determined by comparing many possible models







Phase-sensitive small angle neutron scattering, C.F. Majkrzak, K. Krycka, S. Krueger, N.F. Berk, P. Kienzle and B. Maranville, *J. Appl. Cryst.* 47, 780-787, 2014

- Tag(s) should be asymmetric in X,Y,Z dimensions for maximum phase retrieval
- Tags must attach at same point on objects of interest (one-to-one)
- Tag-Object bond should be “relatively stiff”
- “Sufficient Q range with sufficiently low noise”

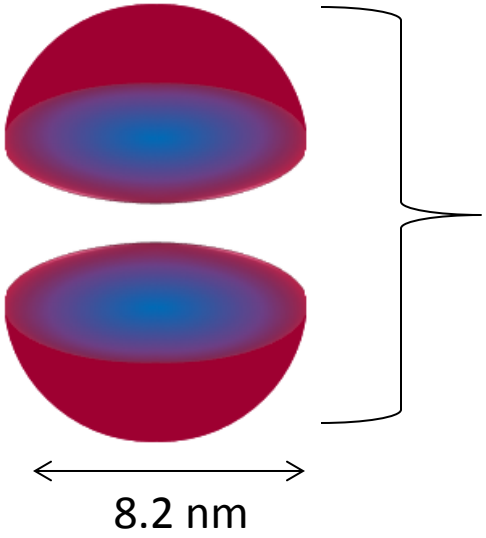
Starting with 1D: Even Core-Shell Morphology Is Difficult To Resolve

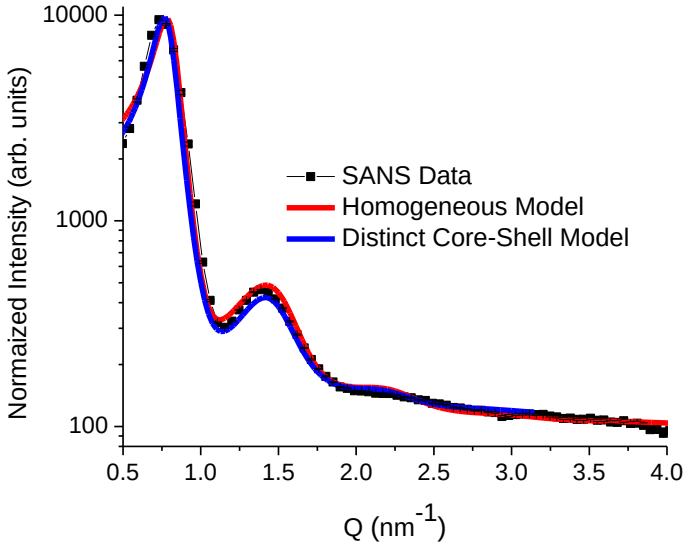
Example:

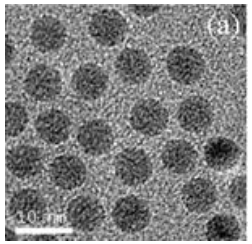
Fe_3O_4
SLD = 6.97×10^{-6} Å^{-1}

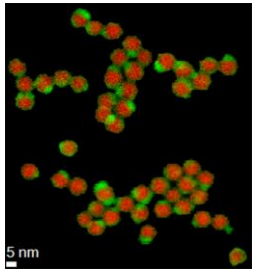
Υ-Mn_2O_3
SLD = 1.71×10^{-6} Å^{-1}

More than a factor of 4 different!

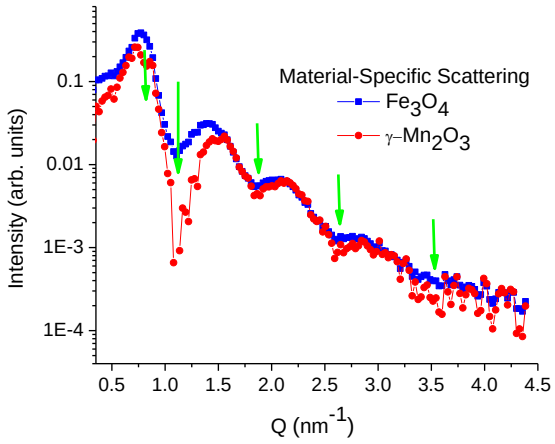


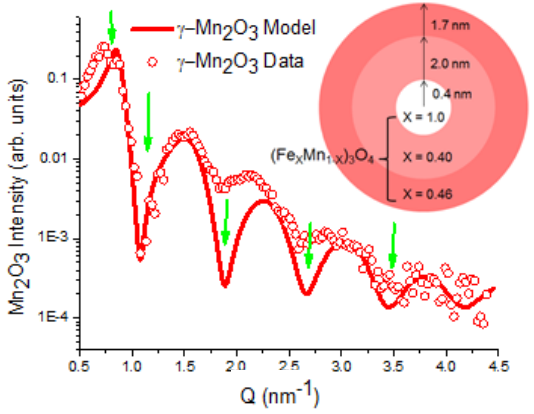






Obtain *phase information* from resonant x-ray scattering:





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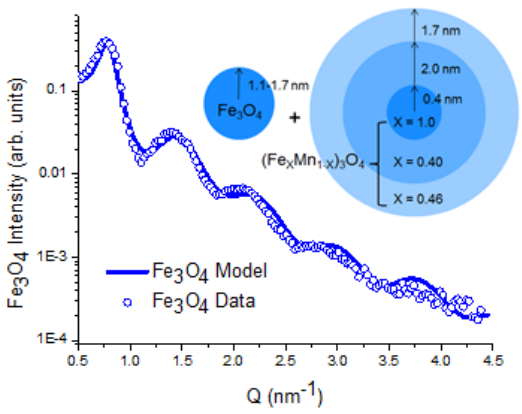
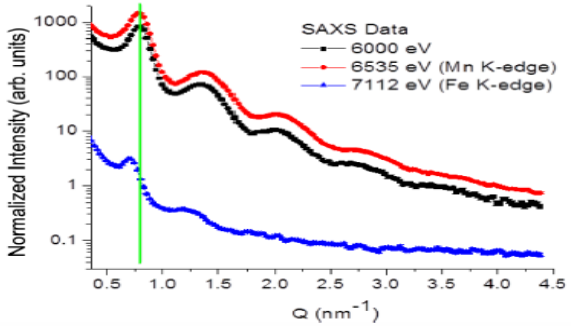


Details in ACS Nano 7, 921-931 (2013)

Ways to Recover Phase

1. Resonant X-ray Scattering
(typically won't remove angular averaging)



2. H-D substitution of solvent
(neutrons, angular averaging still an issue)

3. Isomorphic substitution
(x-ray or neutron, question about changing sample, typically applied to powder or single crystals)

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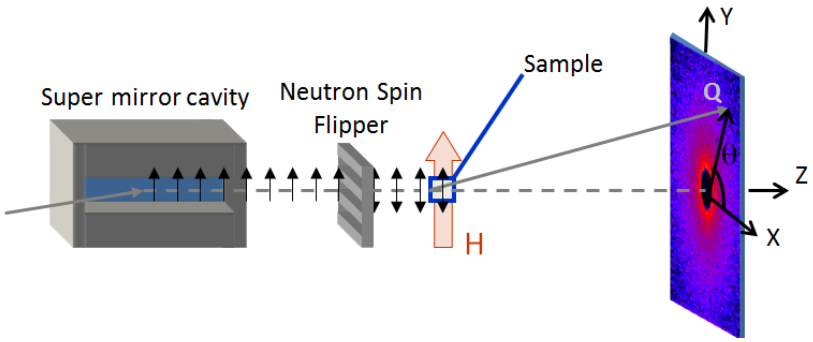
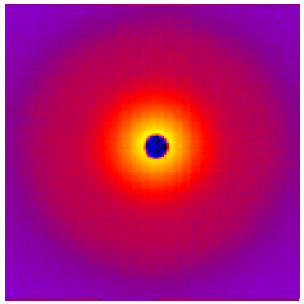
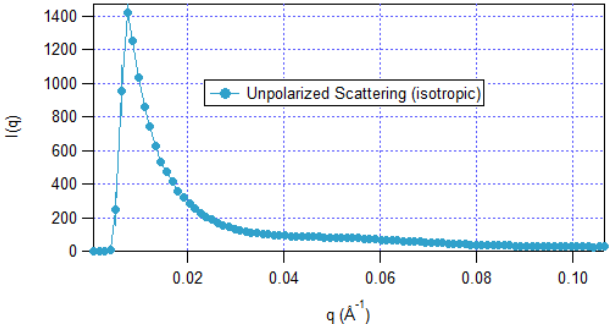
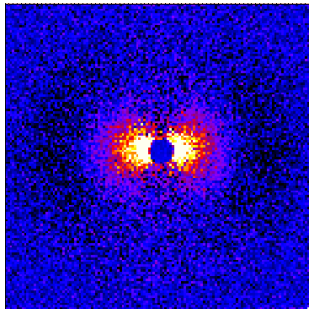
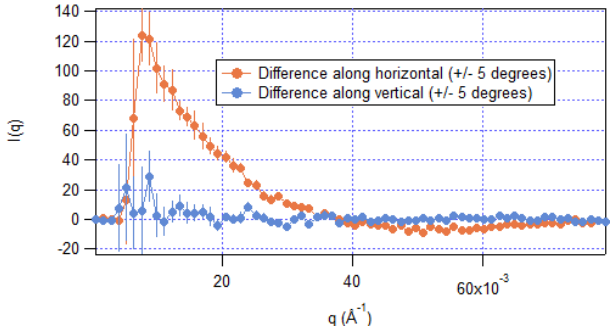
4. <u>Single-sample</u> magnetic reference tag with polarized neutron beam







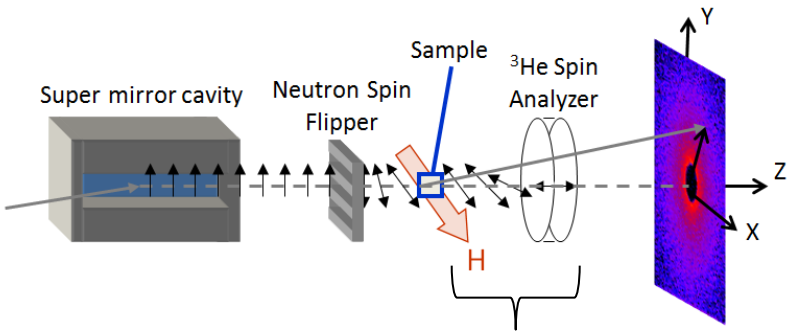




- ↑,↓ *difference* (Nucl-Mag C.T.) eliminates background!
- Neither polarization of optics nor sample saturation need to be perfect in order for this to work.

Recovering Phase with Magnetic Tag

Full-Polarization w/ any magnetic tags



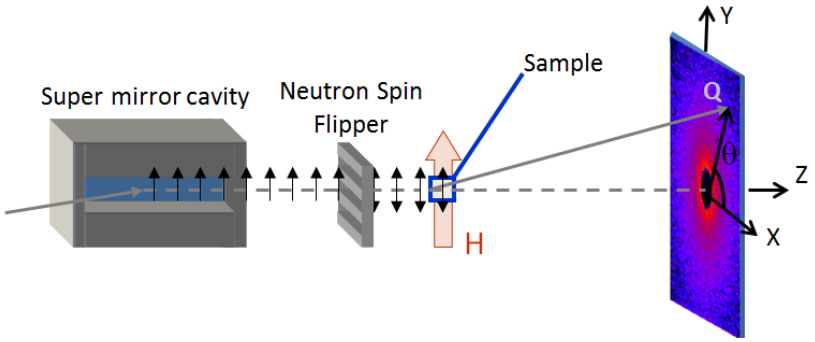
(optional for saturated M)

H || X:

$$\sigma^{\downarrow\downarrow}_{\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q}) = N(\mathbf{Q})N^*(\mathbf{Q}) + M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})\sin^4(\theta)$$
$$+ M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})\cos^2(\theta)\sin^2(\theta)$$
$$- [M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})$$
$$+ M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\sin^3(\theta)\cos(\theta)$$
$$\pm [N(\mathbf{Q})M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q}) + N^*(\mathbf{Q})M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\sin^2(\theta)$$
$$\mp [N(\mathbf{Q})M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q}) + N^*(\mathbf{Q})M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\sin(\theta)\cos(\theta)$$

$$\sigma^{\downarrow\uparrow}_{\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q}) = M_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})$$
$$+ M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})\cos^4(\theta)$$
$$+ M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})\sin^2(\theta)\cos^2(\theta)$$
$$- [M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})$$
$$+ M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\sin(\theta)\cos^3(\theta)$$
$$\pm i[M_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})$$
$$- M^*_{x,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\sin(\theta)\cos(\theta)$$
$$\mp i[M_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M^*_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q}) - M^*_{y,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})M_{z,\hat{\mathbf{p}}_x\perp\hat{\mathbf{n}}}(\mathbf{Q})]\cos^2(\theta)$$

Half-Pol w/ saturated magnetic tags



H || Y:

$\sigma^{\downarrow,\uparrow} = NN^* + M_{||H}M_{||H}{}^*\cos^2(\theta)$
$+,- [NM_{||H}{}^* + N^*M_{||H}]\cos(\theta)$

1) $NM_{||H}$ is Nuclear-Magnetic Cross Term which provides the phase information for N

2) Choose coordinates so M (tag) is *real*

3) Only sensitive to objects *coherent* with magnetic tags in the ↓ - ↑ difference

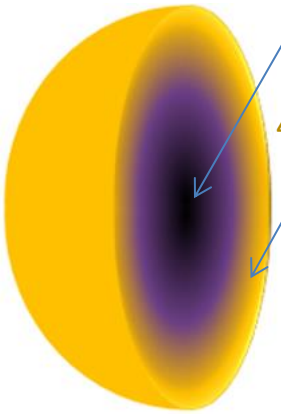
4) Polarizing mirror ~80% transmission for preferred spin state; polarization > 99%

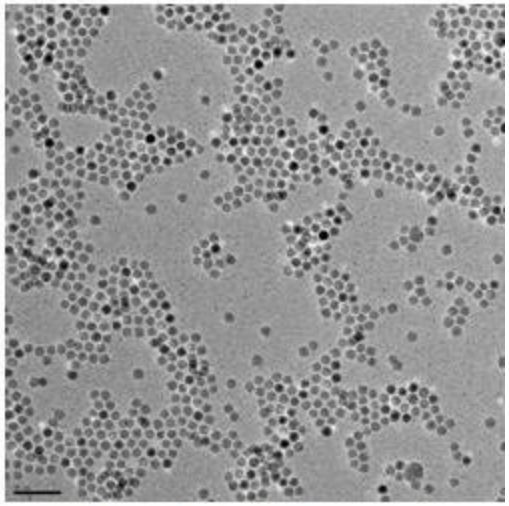
Project Steps for SANS Tagging + Inversion

- Characterize magnetic tags in solution
  - will incoherent hydrogen scattering be problematic?
  - is dilute limit too weak?
  - does chaining occur at saturating magnetic fields?
- Invert core-shell system (1D) with included magnetic component
  - what minimum Q do we need to reach for a given real-space resolution?
  - what statistical signal:noise is needed?
  - focus on simulation versus experimental data comparisons
- Attempt to invert core-shell + attached protein with magnetic component
- (Future) Anisotropic tagging schemes
  - multiple spherical attachments
  - single / multiple nanorods
  - rectangular, layered block (single attachment / protein)
- (Future) Anisotropic attachment
  - oriented Au pads

1D Core-Shell Starting Systems

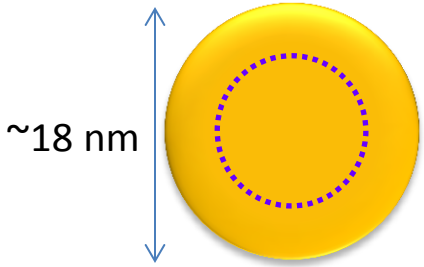
Commercially available from Ocean NanoTech:





TEM of 10 nm Iron Oxide

Catalog number:	IPG-10-01
Product name:	Iron oxide nanoparticles with protein G
Solvent:	Borate (0.05M, pH 7.4) with 1 mg/mL BSA, 0.02% NaN_3
IO size by TEM:	10 nm
Size tolerance:	2.5 nm
Functional group:	Protein G
Storage:	4°C; Do not freeze
pH stability:	4-10
Buffer stability:	Borate, Tris, HEPES, PBS, etc.
Shelf life:	3 months
Volume:	1 mL
Concentration:	1 mg/mL (Fe)
Concentration:	0.86 nmole/mL (nanoparticles)



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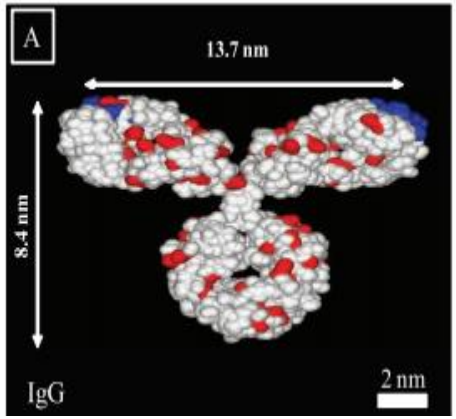

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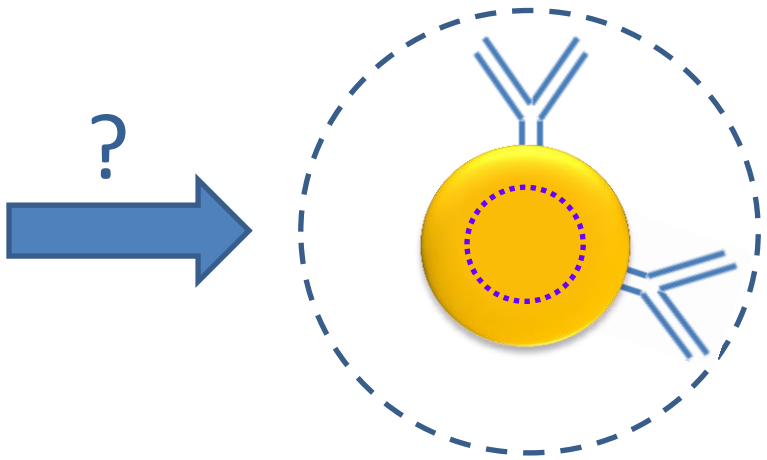
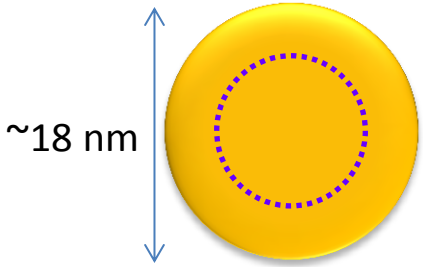
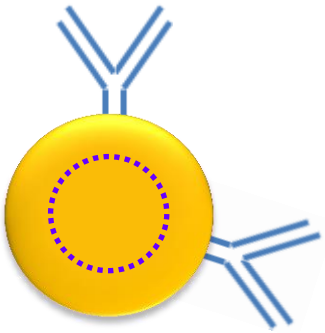


Preparation and characterization of samples

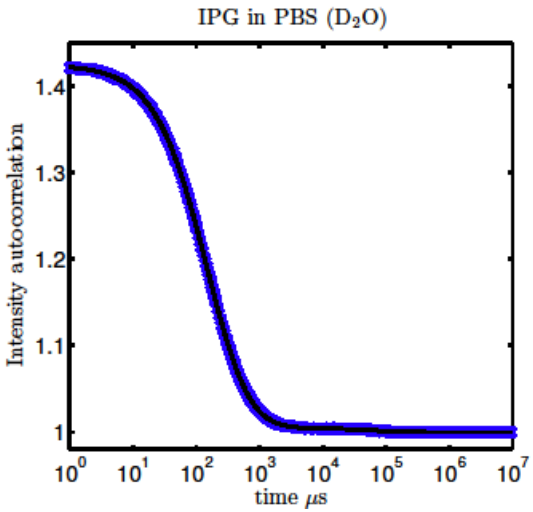
IPG particles:
Stable suspension
Relatively monodisperse
DLS gives small particle size

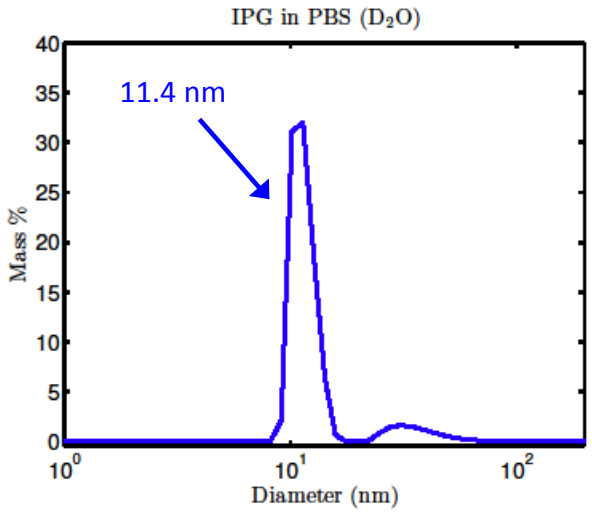


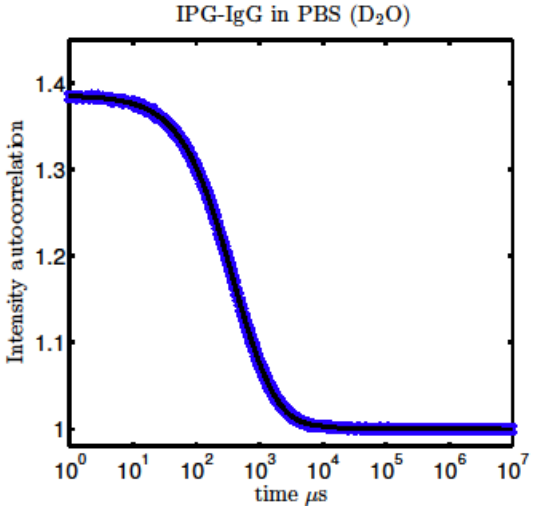
IPG particles – IgG antibodies:
Stable suspension
Relatively monodisperse
No large aggregates

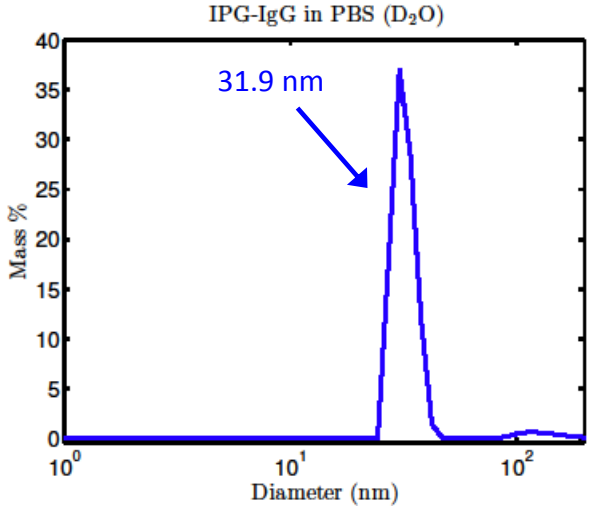


Dynamic light scattering

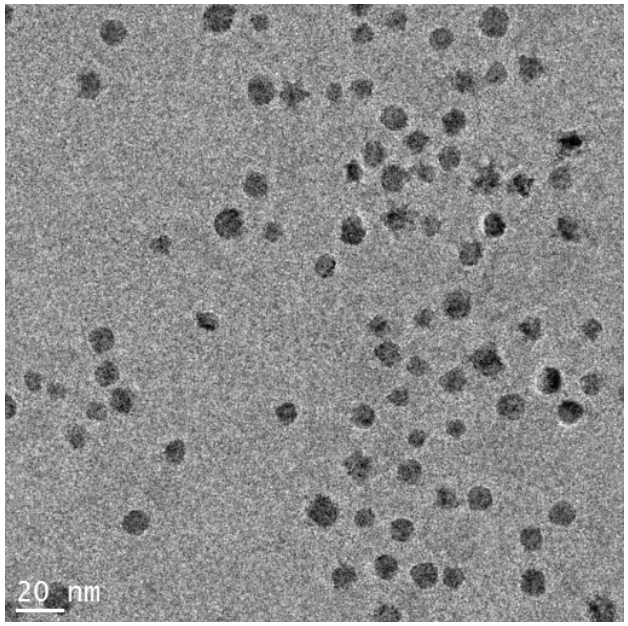








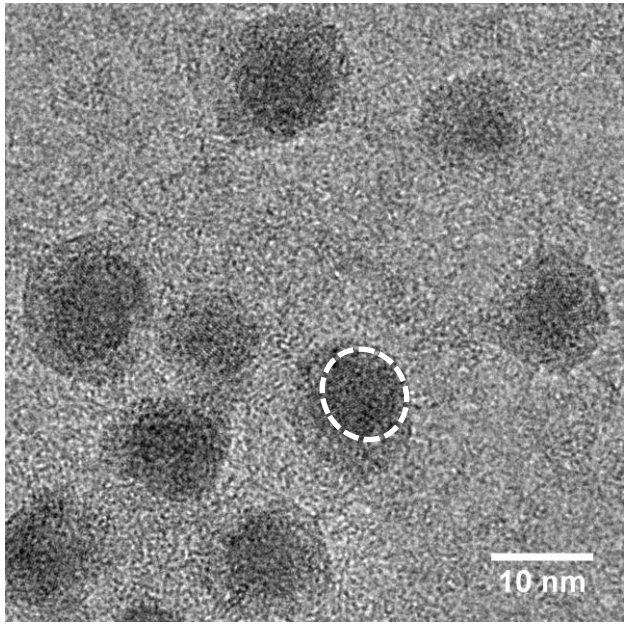
TEM characterization of IPG particles



Well dispersed

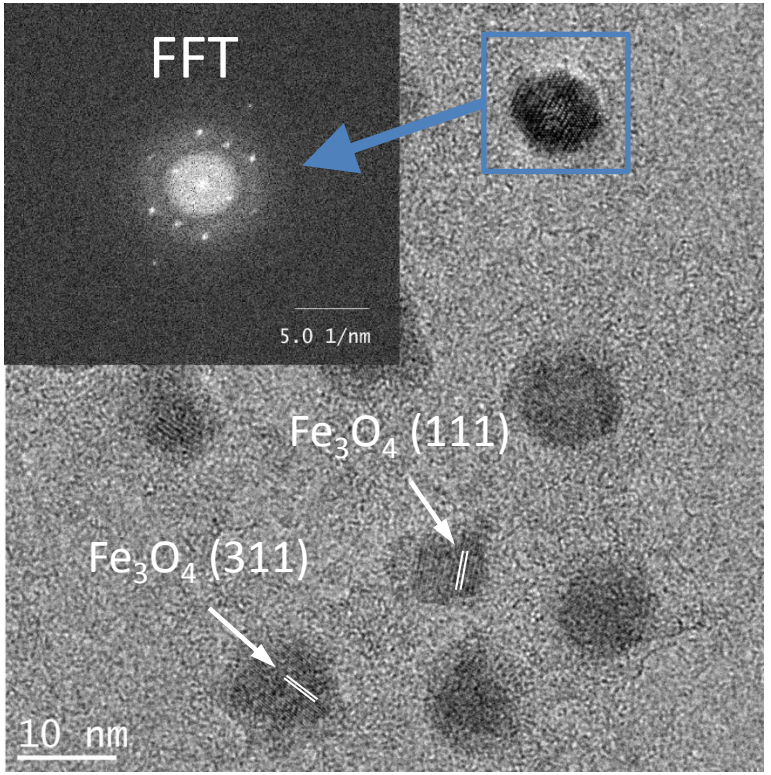
Monodisperse

Spherical



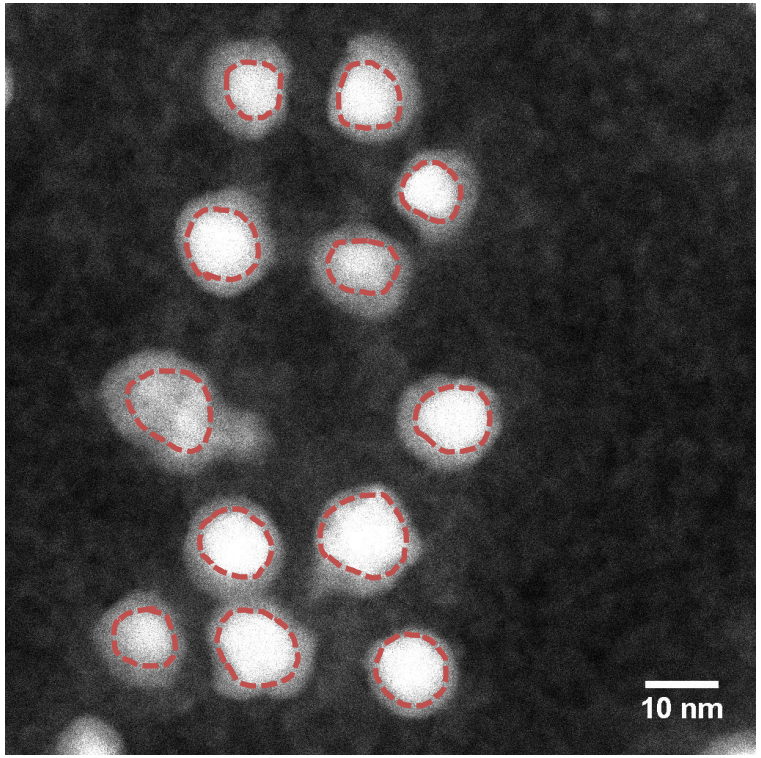
≈ 10 nm core
≈ 2-5 nm shell

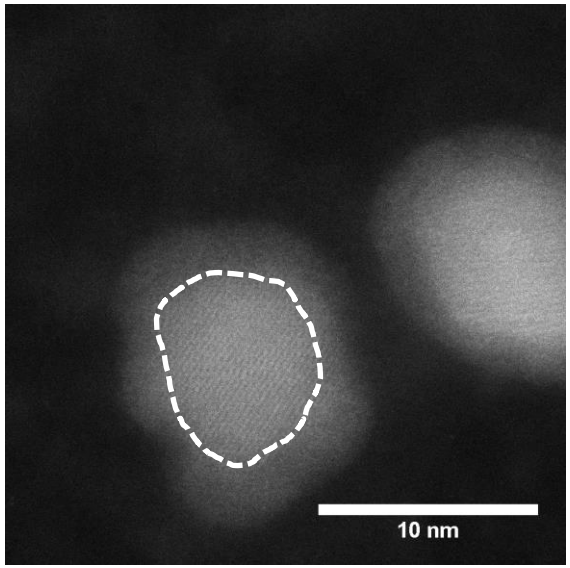
Fe_3O_4 crystal structure

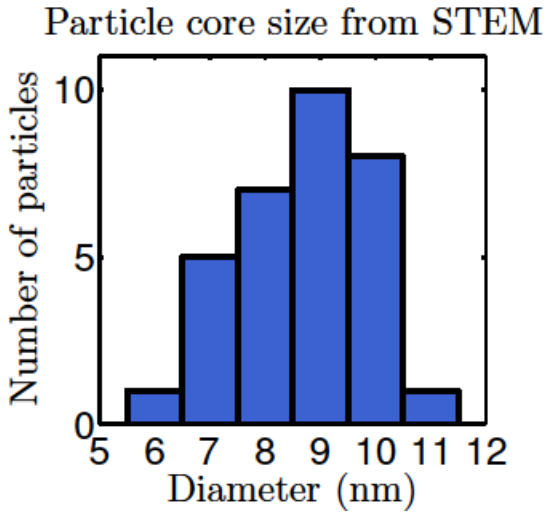


STEM characterization of IPG particles

Core/shell contrast more clear in STEM





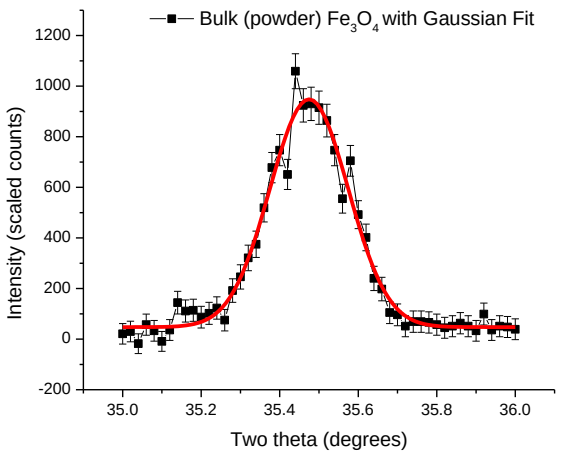


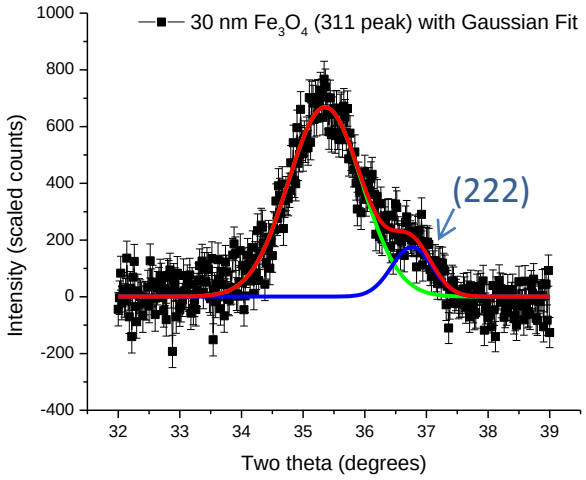
Average core size 8.9 +/- 1.3 nm

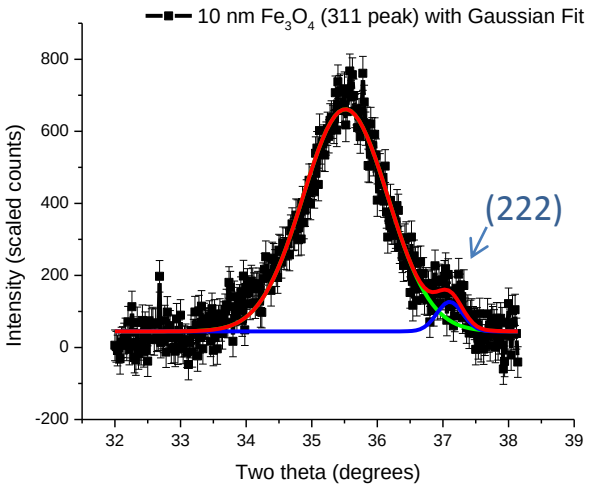
Other characterization methods

- Dynamic light scattering (hydrodynamic size)
- SAXS (particle core)

Magnetic Core Characterization : X-Ray Diffraction (sister samples)





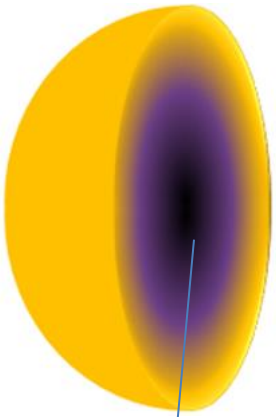


$L = \lambda / FWHM\ (radians) * \cos(2\theta)$

10 nm (FWHM 1.287°) -> 8.4 nm
30 nm (FWHM 1.166°) -> 9.3 nm

In both cases, crystalline size < magnetic core diameter (see next slide).
Nanoparticles appear to be comprised of multiple crystalline grains.

1D Case: Core-Shell Morphology, Basic Magnetic Characterization



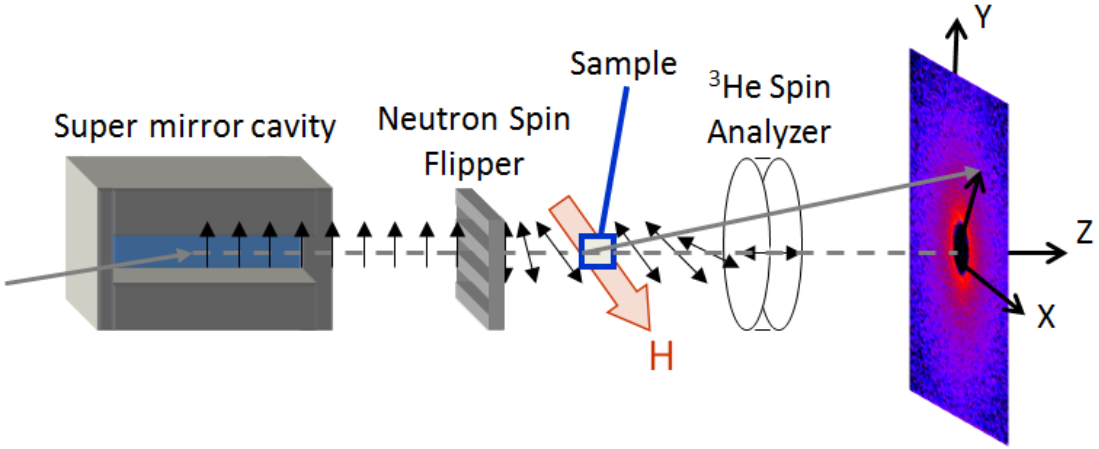
~10 nm diameter Fe_3O_4
$\Delta SLD = 0.58 \times 10^{-6}$ Å^{-1}

4-5 nm thick Protein G
$\Delta SLD = -2.0 \times 10^{-6}$ Å^{-1}

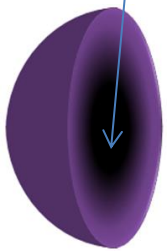
D_2O Buffer
Δ SLD = 0.0×10^{-6} Å^{-1}

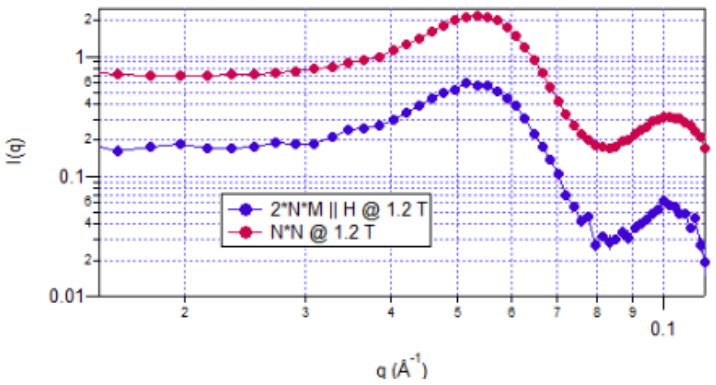
Dilute Solution
~1mg/mL

"Full Polarization" at 0.005 T and 1.2 T

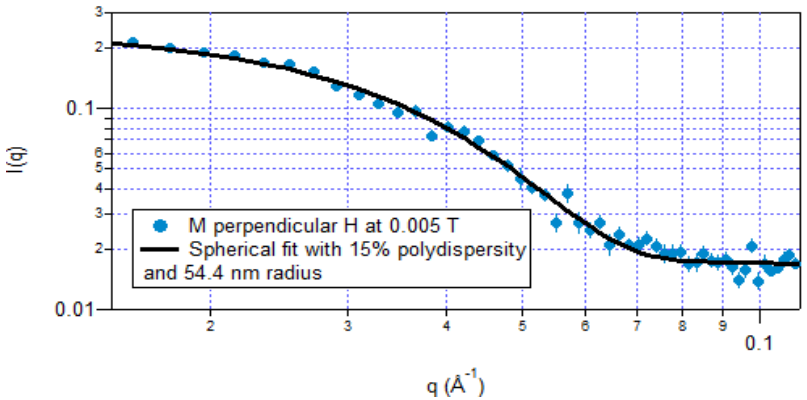


'5% Polydisperse' within batch Ocean NanoTech Nanoparticles. Examine similar batch (~10 nm diameter, dried) Fe_3O_4 cores with thin oleic acid cap to determine diameter and magnetic signal. Thanks to SURF student, Henry Le.



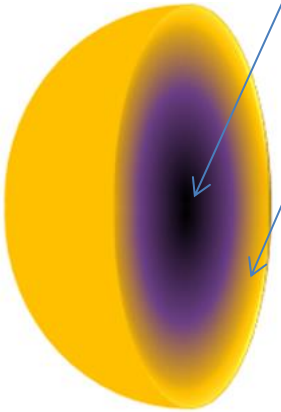


75% as magnetic as bulk Fe_3O_4 at saturation, 300 K (magnetic SLD = 1.1×10^{-6} Å^{-1}).



Fitting of magnetic signal at remanence gives *magnetic* 10.8 nm diameter, PD = 10-15%

1D Case: Core-Shell Morphology With Magnetic Reference



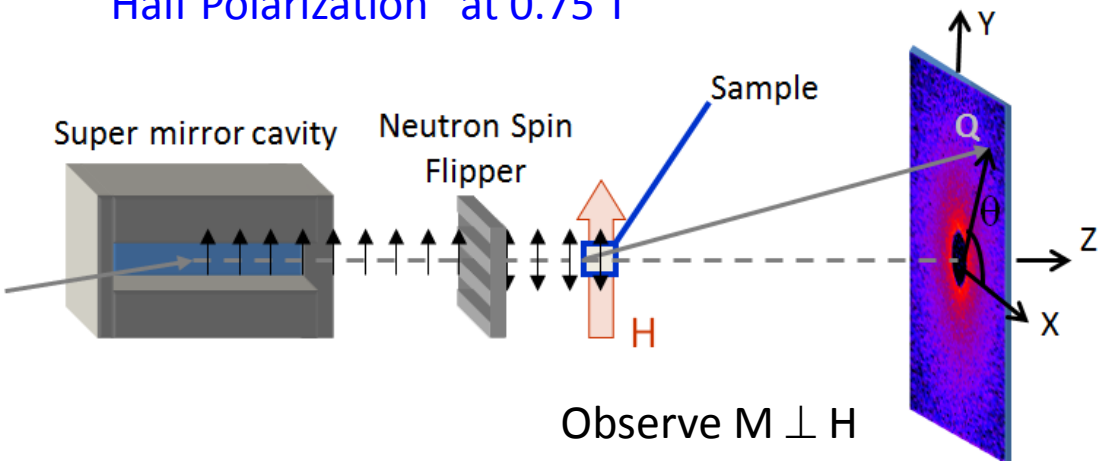
~10 nm diameter Fe_3O_4
$\Delta SLD = 0.58 \times 10^{-6}$ Å^{-1}

4-5 nm thick Protein G
$\Delta SLD = -2.0 \times 10^{-6}$ Å^{-1}

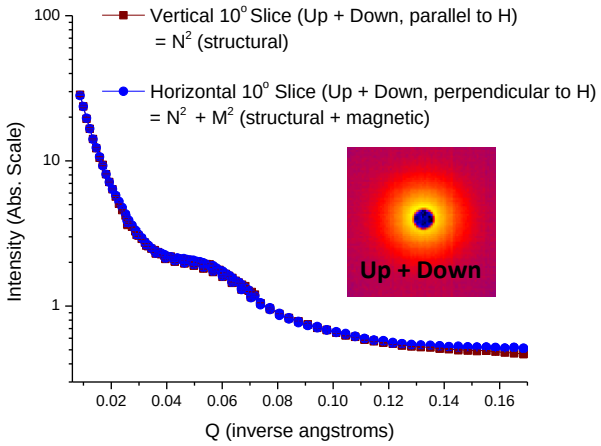
D_2O Buffer
Δ SLD = 0.0×10^{-6} Å^{-1}

Dilute Solution
~1mg/mL

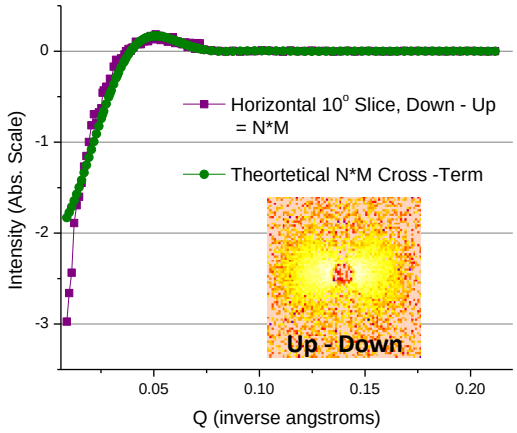
"Half Polarization" at 0.75 T

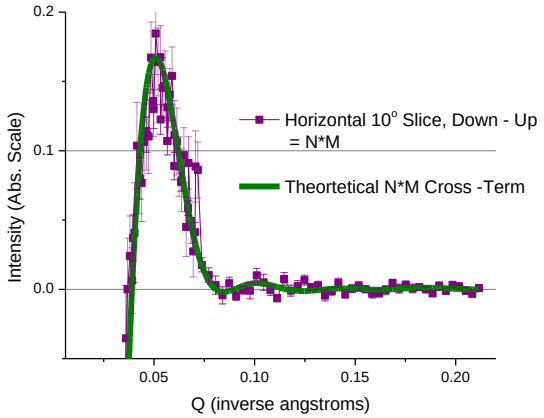


Observe M ⊥ H



(1) No apparent chaining due to field
(2) Hard to detect M^2

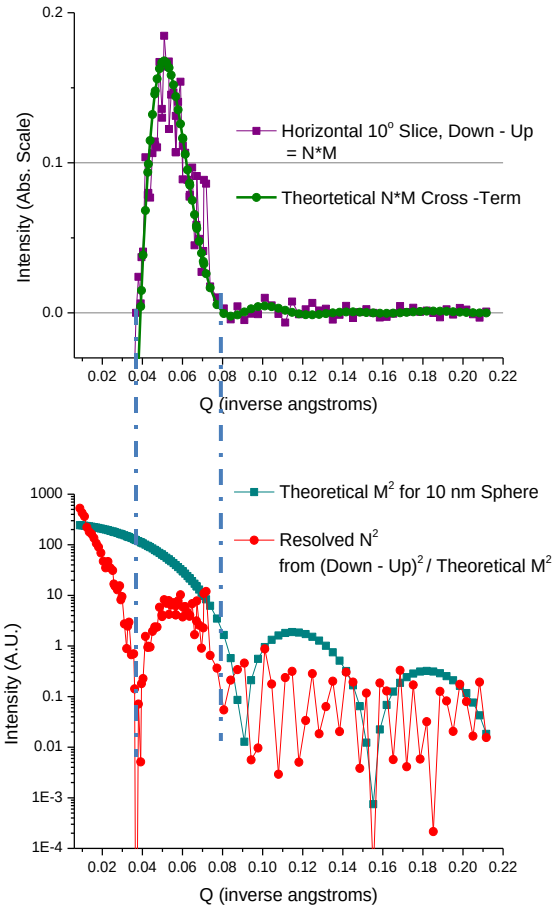


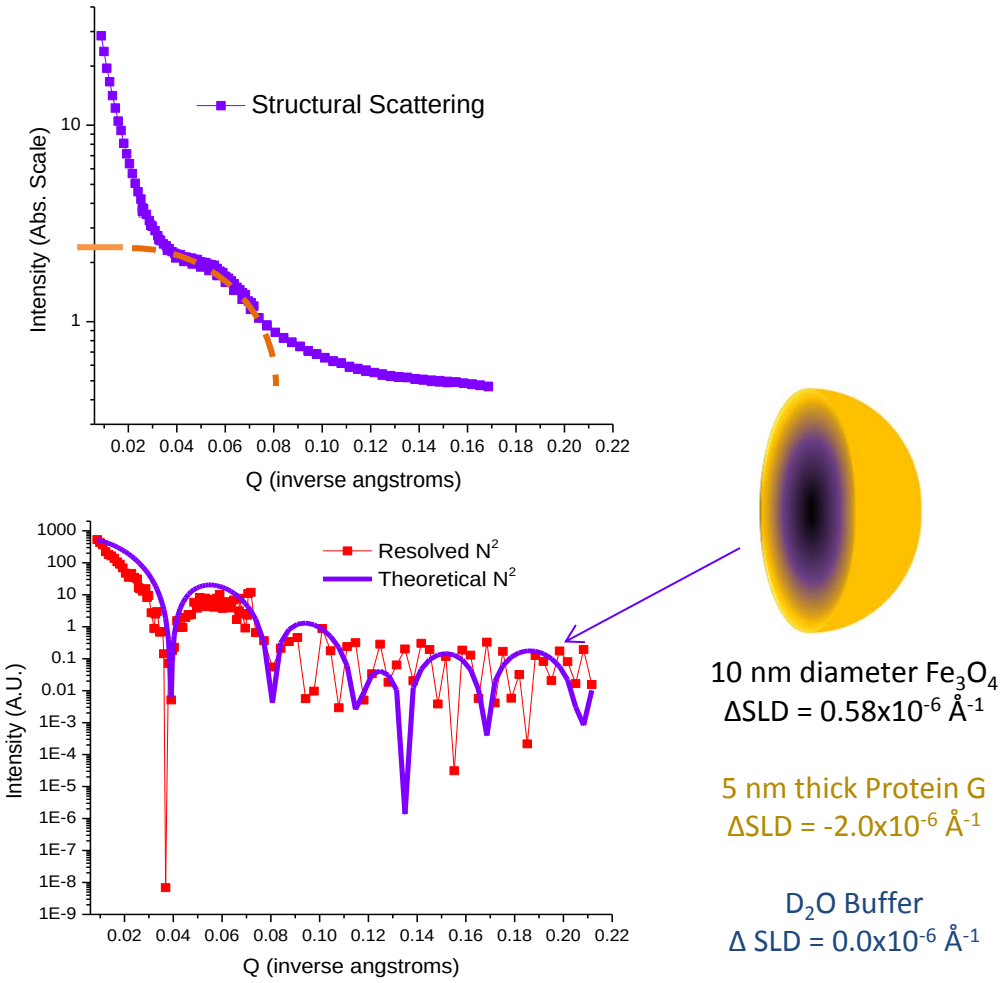


(1) N*M signal is robust (12 hours @ 4m, 12 hours @ 1m)
(2) Low-Q lenses not possible with pol-beam (USANS, VSANS)
(3) High-Q currently truncated by magnet shielding
(4) Note that difference signal completely removes incoherent noise!

1D Case: Quick and Dirty Check (point-by-point analysis)

$N^2 \propto (\downarrow - \uparrow)^2$ / (known M scattering) = $(NM)^2$ / M^2





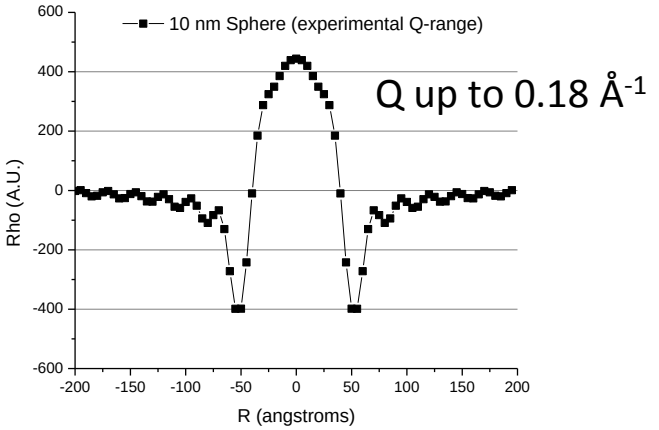
- Zero crossings in difference correlate to resolved N^2 dips (<u>20 nm total diameter</u>)
- Resolved N^2 is very different from M^2

- N^2 details are not easily resolved from unpolarized measurement (top)
- Theoretical and resolved N^2 are very similar

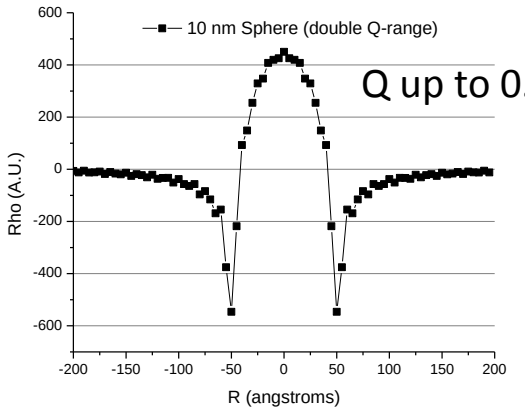
1D Case: Inversion (*Real* nuclear amplitude = Fourier sum of cosines)

1) Since scattering from magnetic reference tag is real, NM*+N*M only selects for real component of nuclear scattering amplitude
2) $N_{amplitude(real)} = \Sigma_n \rho_n [e^{iQ\cdot Rn}]_{real} = \Sigma \rho_n \cos(Q\cdot R_n)$
3) $\rho_n \approx 2/\pi \Sigma_Q N_{amplitude} \cos(Q\cdot R_n) \Delta Q$

Theoretical Inversions From 50 Å Radius Sphere



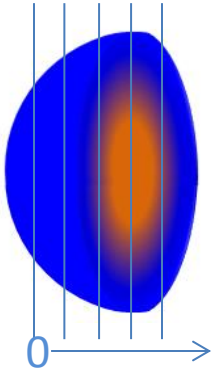
Q up to 0.18 Å^{-1}



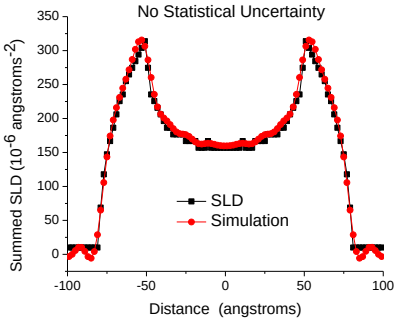
Q up to 0.36 Å^{-1}

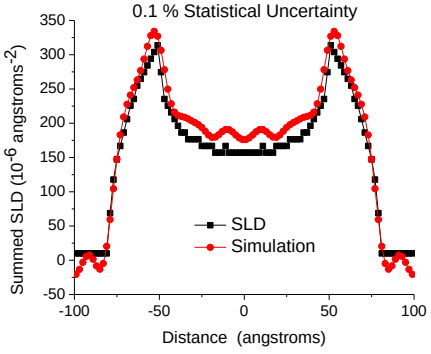
Ringing at sharp interface edge is expected, especially for finite Q

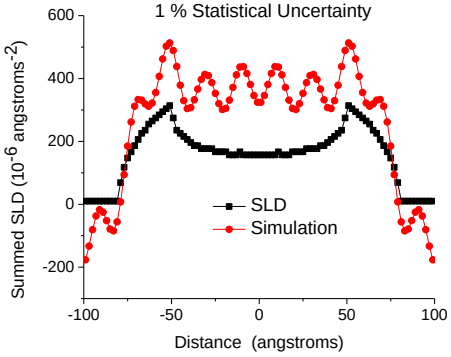
"Infinite" Q



Core-Shell Model (cross-section)







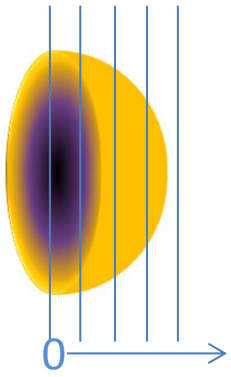
1D Case: Inversion (*Real* nuclear amplitude = Fourier sum of cosines)

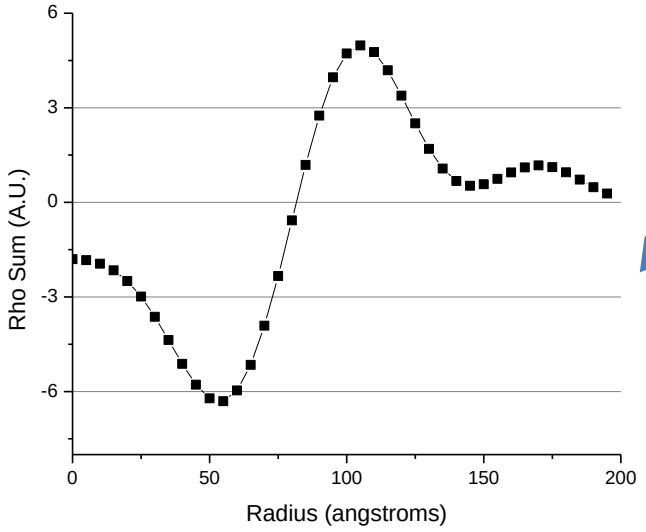
Theoretical Inversions (simulation with inversion with Q range similar to experiment)

~10 nm diameter Fe_3O_4
$\Delta SLD = 0.58 \times 10^{-6}$ Å^{-1}

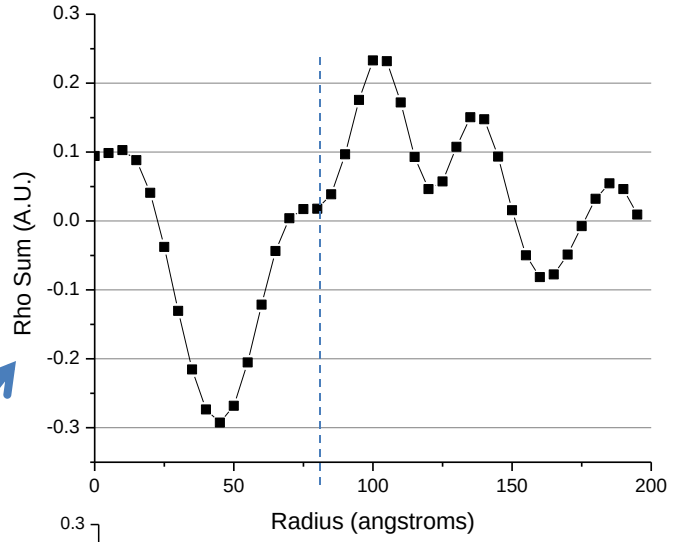
4-5 nm thick Protein G
$\Delta SLD = -2.0 \times 10^{-6}$ Å^{-1}

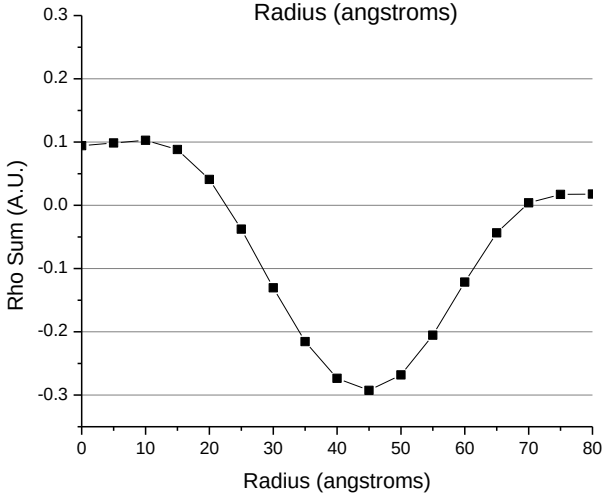
D_2O Buffer
Δ SLD = 0.0×10^{-6} Å^{-1}





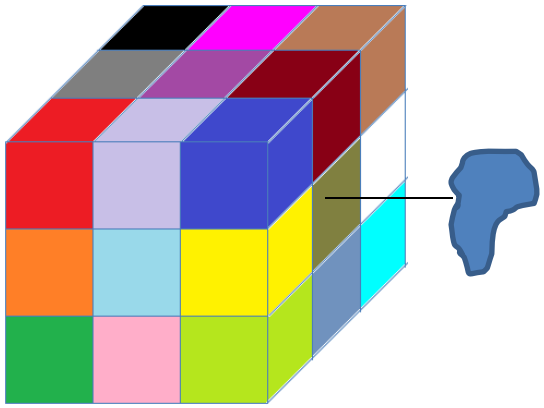
Experimental Inversion from Down – Up Difference (assuming 50 Å magnetic core radius)



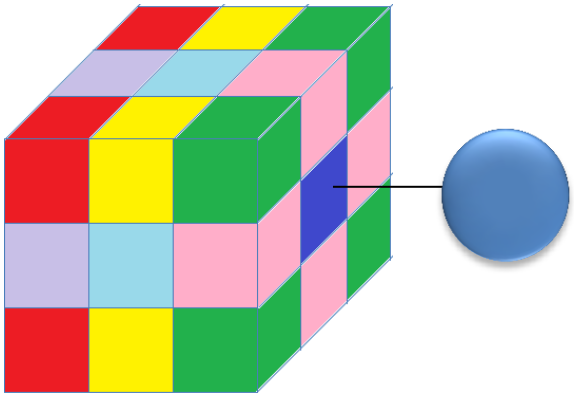


Oscillations are an issue, but profile is plausible and suggestive of a thinner (or less dense) protein shell

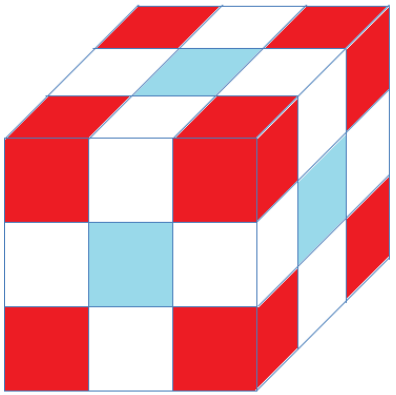
1D Case: Inversion in *Spherical Coordinates*



Asymmetric tag

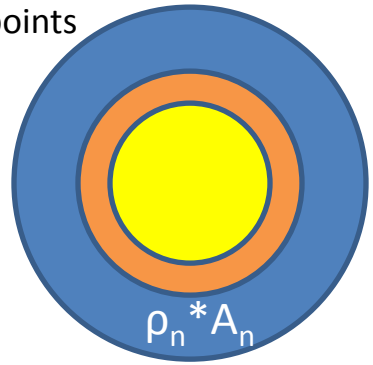


Spherical tag with offset



Centro-symmetric spherical tag

n radial slices
m q-points



$$\begin{pmatrix} A1(q1) & \dots & An(q1) \\ & \dots & \\ A1(qm) & \dots & An(qm) \end{pmatrix} \begin{pmatrix} \rho 1 \\ \dots \\ \rho n \end{pmatrix} = (Diff(q1) \;\; Diff(q2) \;\; \dots Diff(qm))$$

Matrix A (defined)

Matrix ρ (to solve)

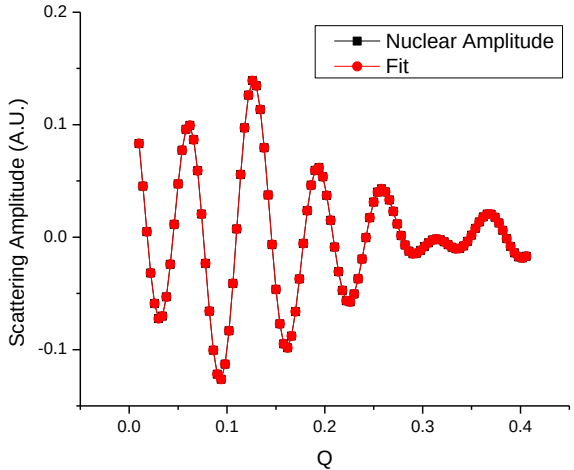
Matrix D (measured) = Nucl-Mag C.T. / 'known' Mag. Amplitude

$$\rho = (A^T A)^{-1} A^T D$$

$A_n(Q) \propto [(\sin(Q*R_n)-Q*R_n*\cos(Q*R_n))-(\sin(Q*R_{n-1})-Q*R_{n-1}*\cos(Q*R_{n-1}))] / Q^3$

1D Case: What would it take to achieve 1 nm resolution?

Radius (nm)	Actual_Rho	Rho from Q to 0.4 Å^{-1}	Rho from Q to 0.3 Å^{-1}	Rho from Q to 0.25 Å^{-1}	Rho from Q to 0.2 Å^{-1}
1	0.5	0.499795	0.501387	4.27271	236.184
2	1.0	1.00005	0.999361	-0.598791	-74.8248
3	2.0	1.99999	2.00043	2.92414	21.3793
4	-2.0	-1.99995	-2.00036	-2.5892	5.38521
5	-3.0	-3.00011	-2.99967	-2.61324	-21.3067
6	5.0	5.0001	4.99976	4.74727	24.6038
7	0.1	0.099975	0.100162	0.260844	-15.7318
8	4.0	3.99996	3.99985	3.9021	14.4677
9	-9.0	-8.99992	-8.99982	-8.94425	-14.7146
10	-5.0	-5.00011	-5.00016	-5.02878	-2.4993
11	8.0	8.00008	8.00007	8.01252	7.19414
12	0.3	0.299975	0.299993	0.296701	0.445809

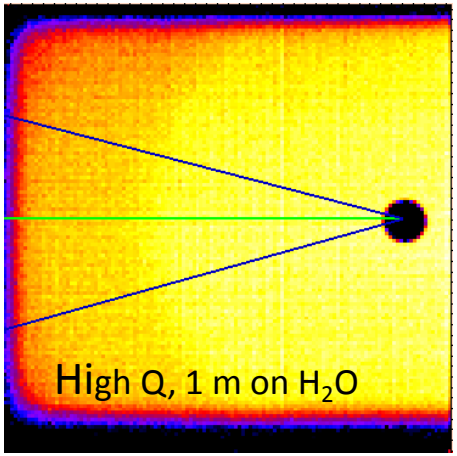


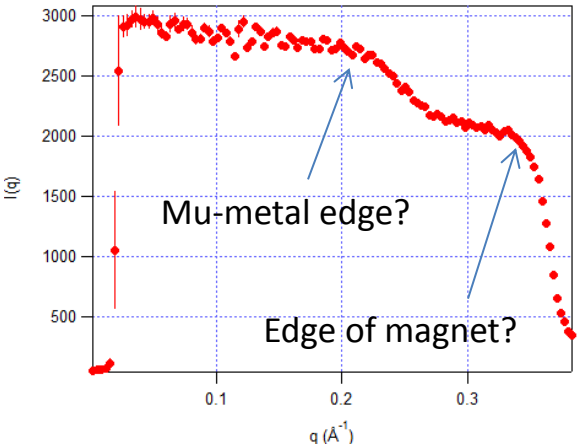
Rule of minimum q needed ~2π/feature size
Example: π/(2*radius) = 2π/20 Å = 0.31 Å^{-1}

Experimental 0.18 Å^{-1} -> ~35 Å minimum (18 Å inner radius)

If signal drops ~0.12 Å^{-1} -> ~50 Å minimum (25 Å radius) ?

1D Case: What resolution is appropriate for our experiment?





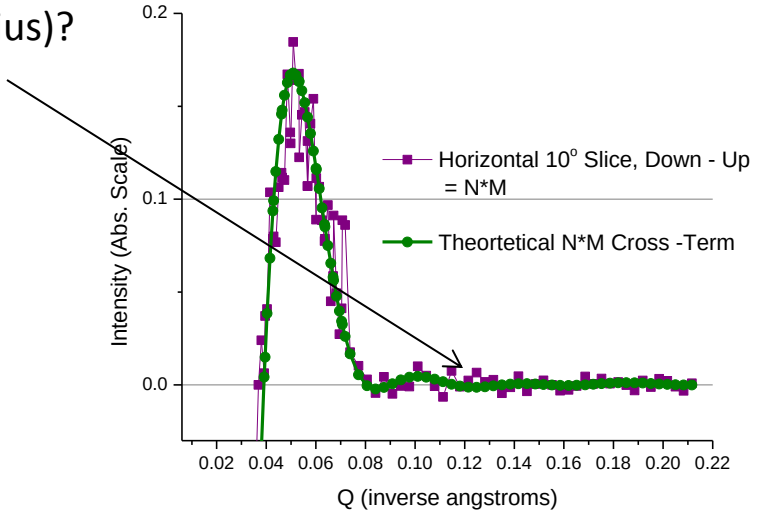
SASCALC predicts 0.44 Å^{-1} without magnet at Huber position and 0.64 Å^{-1} at sample chamber. However, we also want a moderate field of about 0.5 T.

Experimental 0.2 Å^{-1} -> ~31 Å minimum (16 Å inner radius)

If signal drops ~0.12 Å^{-1} -> ~50 Å minimum (25 Å inner radius)?

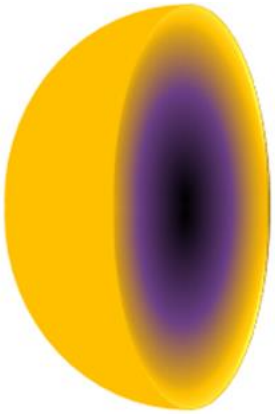
A reasonable range might be for Q up to 0.12 Å^{-1}:

Radii(Å)	Input Rho	Inverted Rho
30	0.5	0.506635
40	-2.0	-2.0186
50	1.0	1.01321
75	-3.0	-3.00165
100	5.0	5.00067
110	1.5	1.49926
150	0.1	0.10003



1D Case: Simulating Experiment (check of magnetic core and diameter)

Simulate Nucl-Mag C.T. and Mag. Ampl.:



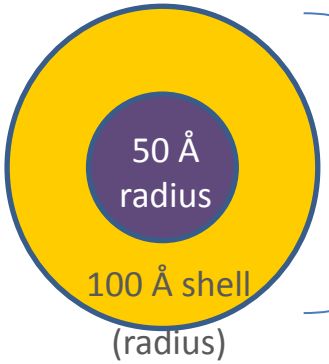
10 nm diameter Fe_3O_4
MSLD = 1.46×10^{-6} Å^{-1}

10 nm diameter Fe_3O_4
ΔSLD = 0.58×10^{-6} Å^{-1}

5 nm thick Protein G
ΔSLD = -2.0×10^{-6} Å^{-1}

D_2O Buffer
Δ SLD = 0.0×10^{-6} Å^{-1}

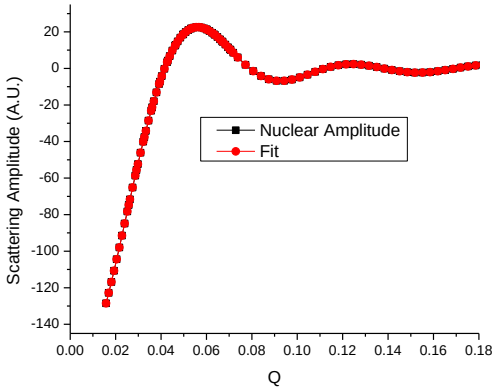
Two-shell (Q matches expt. up to 0.18 Å^{-1})



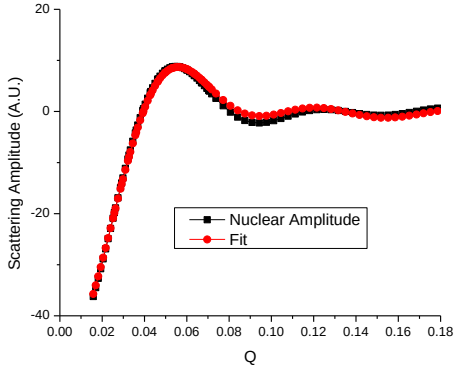
ρ_{inner} = +0.58

ρ_{outer} = -2.00003

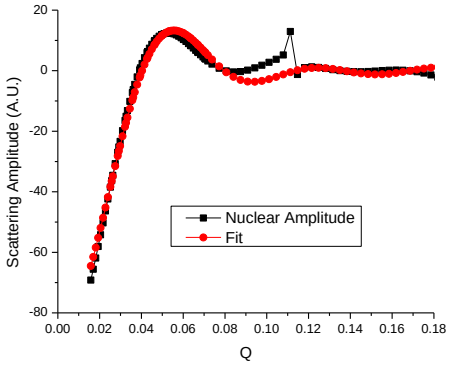
Residual 0.0977



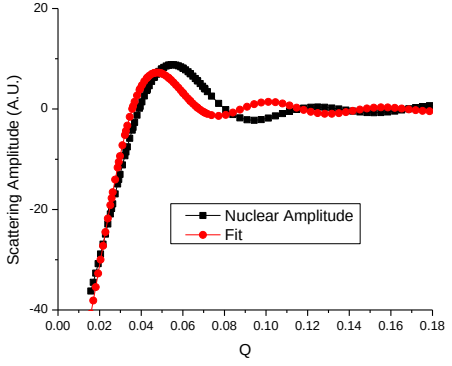
Input (alter internal boundary):
Mag. Radius = 50 Å
Nucl. Core = 40 Å radius -> ρ = 0.58
Nucl. Shell = 100 Å radius -> ρ = -0.592
Residual = 73



Input (shrink mag. core):
Mag. Radius = 40 Å
Nucl. Core = 50 Å radius -> ρ = 0.58
Nucl. Shell = 100 Å radius -> ρ = -39.48
Residual = 273



Input (increase total size):
Mag. Radius = 50 Å
Nucl. Core = 40 Å radius -> ρ = 0.58
Nucl. Shell = 120 Å radius -> ρ = -4.304
Residual = 340



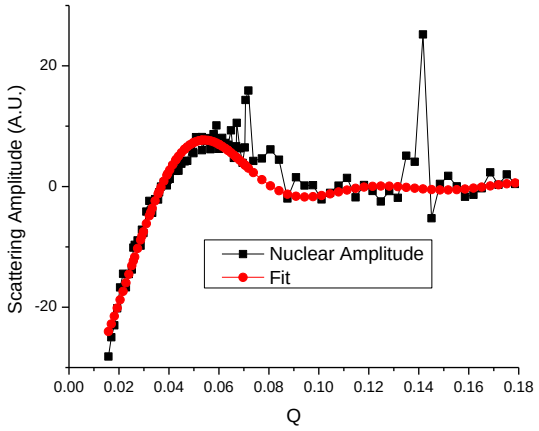
1D Case: Inversion in Spherical Coordinates (Data!)

Can be fairly certain that total nuclear radius is ~9-10 nm; mag. core radius is ~50 Å (company specs)
Q of SANS 0.01579 $Å^{-1}$ to 0.18 $Å^{-1}$

Trial Input (three quadrants):
Mag. Radius = 55 Å
Nucl. Core = 50 Å radius
Nucl. Shell_1 = 100 Å radius
Nucl. Shell_2 = 150 Å radius

ρ_{core} = 0.58 ρ_{shell1} = -0.728
ρ_{shell2} = 0.00265

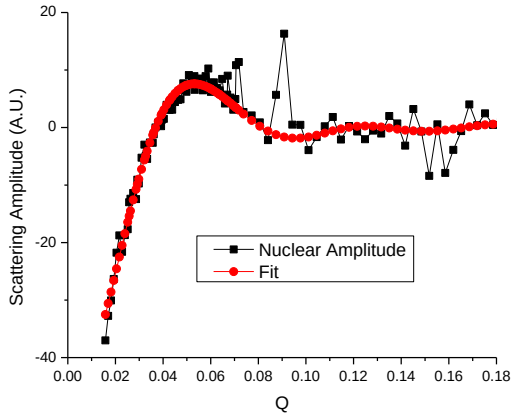
Residual 299



Trial Input (three quadrants):
Mag. Radius = 50 Å
Nucl. Core = 50 Å radius
Nucl. Shell_1 = 100 Å radius
Nucl. Shell_2 = 150 Å radius

ρ_{core} = 0.58 ρ_{shell1} = -1.16549
ρ_{shell2} = -0.069641

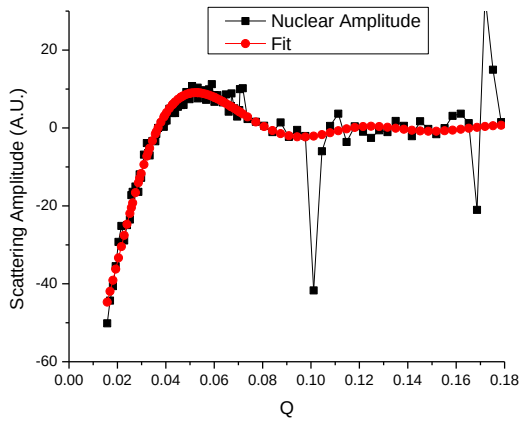
Residual 280



Trial Input (three quadrants):
Mag. Radius = 45 Å
Nucl. Core = 50 Å radius
Nucl. Shell_1 = 100 Å radius
Nucl. Shell_2 = 150 Å radius

ρ_{core} = 0.58 ρ_{shell1} = -1.58535
ρ_{shell2} = -0.14284

Residual 435



Conclusion: Magnetic core 40 to 50 angstroms in radius.

IPG Core-Shell Inversion

Mag. Core = 50 Å radius

"Core"
Radius 30 Å: ρ = 0.316
Radius 40 Å: ρ = 0.580

"Shell"
Radius 50 Å: ρ = -0.431
Radius 75 Å: ρ = -0.230
Radius 100 Å: ρ = -0.127

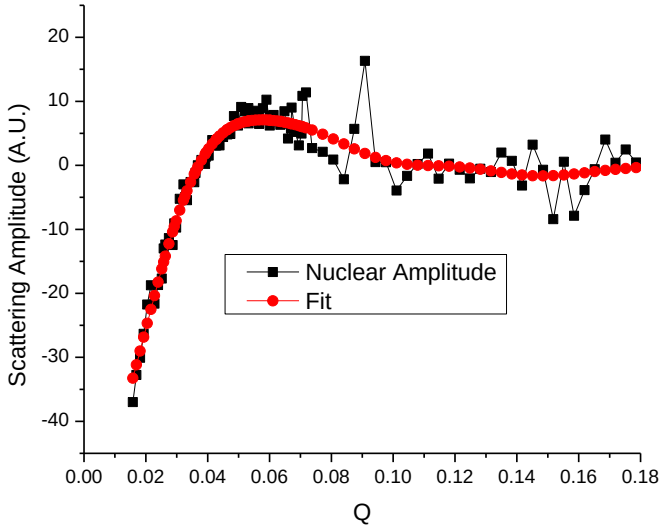
"Solvent"
Radius 110 Å: ρ = -0.022
Radius 150 Å: ρ = -0.022

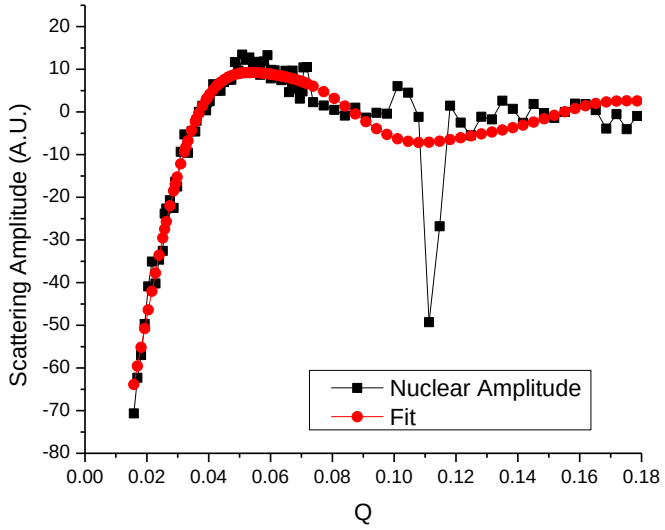
Mag. Core = 40 Å radius

"Core"
Radius 30 Å: ρ = -0.460
Radius 40 Å: ρ = 0.580

"Shell"
Radius 50 Å: ρ = 0.292
Radius 75 Å: ρ = -0.380
Radius 100 Å: ρ = -0.107

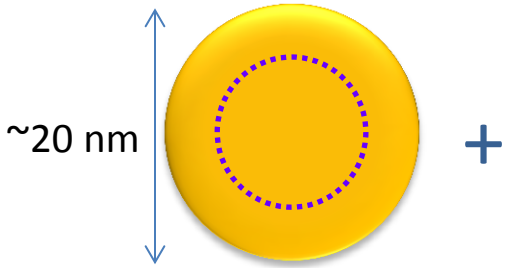
"Solvent"
Radius 110 Å: ρ = -0.044
Radius 150 Å: ρ = -0.034



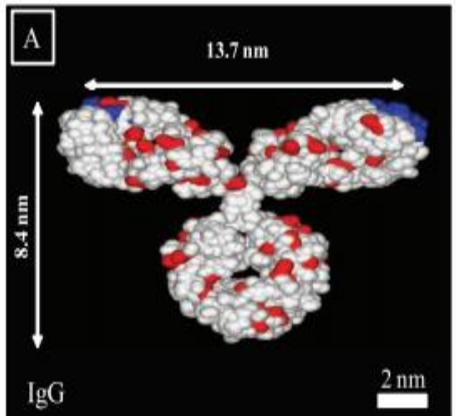


At limit of 40 to 50 Å radius magnetic core. Do see + core, -protein shell, buffer at 100 Å and beyond.

Did we tag IPG core-shell with IgG anti-bodies?



+



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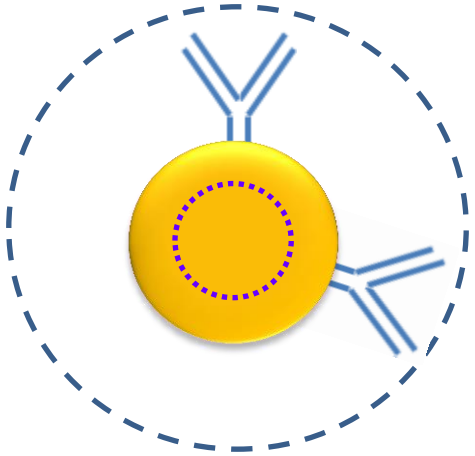
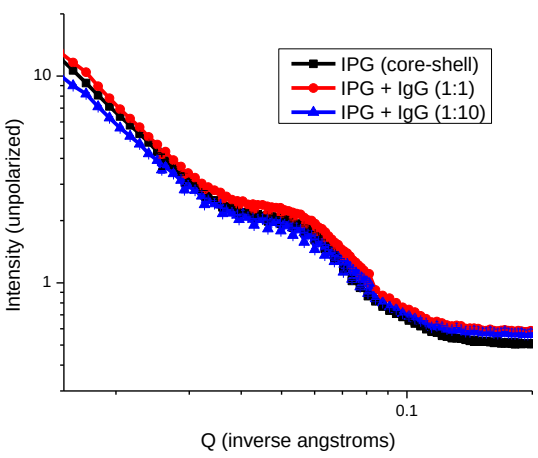
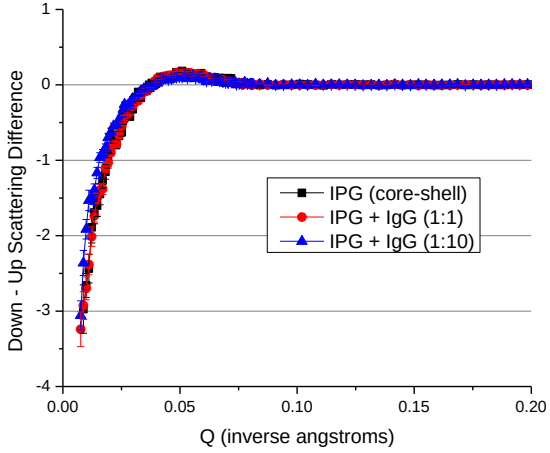
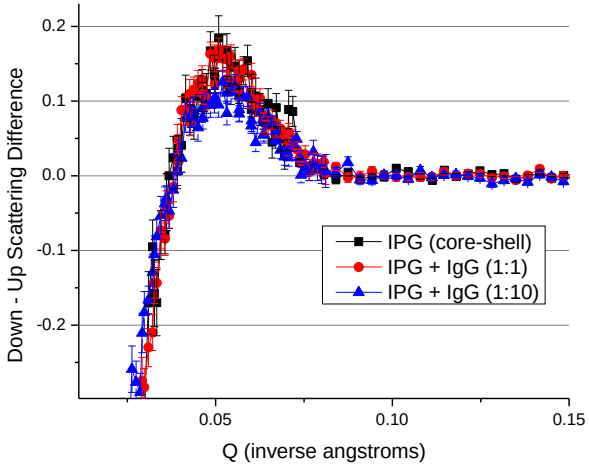
?









Similar zero-crossings of Nucl-Mag C.T. indicate virtually same-sized particles.

IPG + IgG Inversions

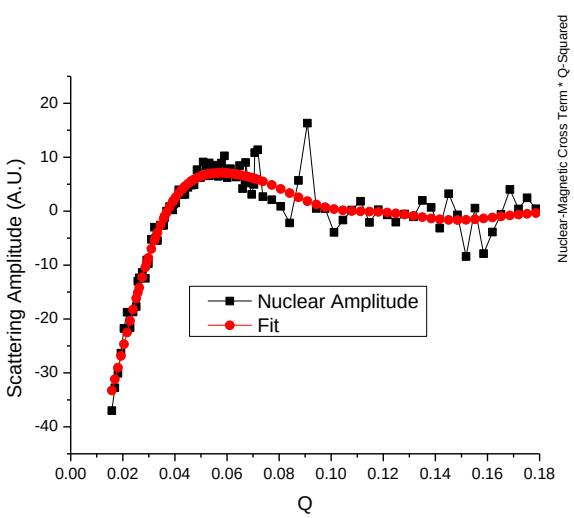
Mag. Core = 50 Å radius

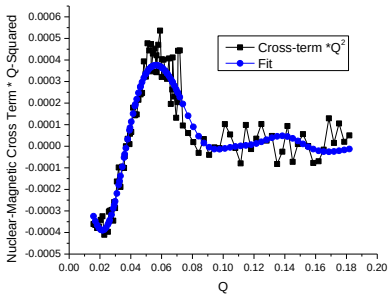
IPG Alone

Radius 30 Å: ρ = 0.316 "Core"
Radius 40 Å: ρ = 0.580

Radius 50 Å: ρ = -0.431
Radius 75 Å: ρ = -0.230 "Protein Shell"
Radius 100 Å: ρ = -0.127

Radius 110 Å: ρ = -0.022
Radius 150 Å: ρ = -0.022 "Solvent"





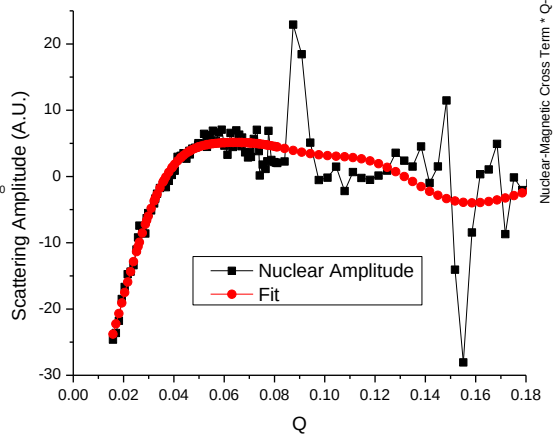
Decent fit

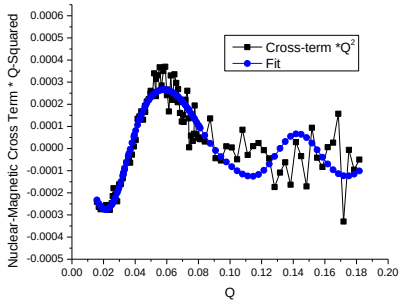
IPG + 10 x's IgG

Radius 30 Å: ρ = 0.194
Radius 40 Å: ρ = 0.580 "Core"

Radius 50 Å: ρ = -0.670 "Protein Shell"
Radius 75 Å: ρ = -0.006

Radius 100 Å: ρ = -0.060
Radius 110 Å: ρ = 0.0031
Radius 150 Å: ρ = -0.0087 "Solvent"





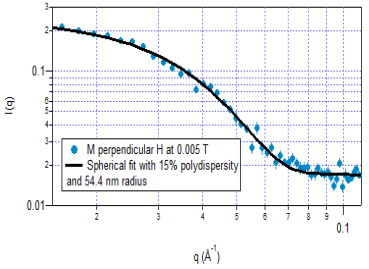
Fit not so great

Conclusion: Data of IPG + IgG is not of sufficient quality (several hours) to distinguish from IPG only.

Recap on Spherical Inversion

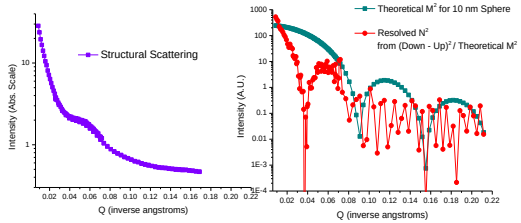
- Using Nuclear-Magnetic cross-term adds additional information to conventional SANS

Pros:	Cons:
~10% polydispersity in spherical magnetic reference OK	Need magnetic reference shape
Can characterize magnetic reference from PASANS →	~50 mg magnetic tags for PASANS
↓-↑ difference eliminates background scattering!	
Partial polarization or partial magnetic saturation OK	



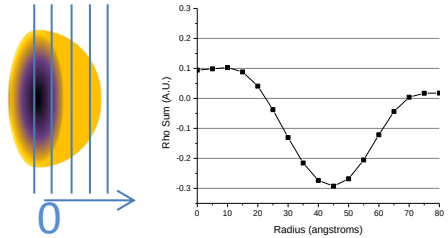
- Point-by-point [$N^2 \propto (\downarrow\text{-}\uparrow)^2$ / (known M scattering)]

Easy to implement on any Q-range	Limited internal sensitivity
Enhanced sensitivity to outer N^2 boundary	



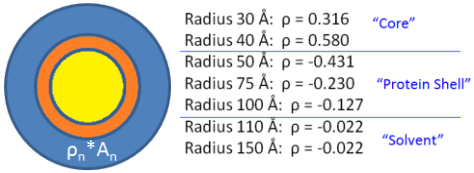
- Inverse Fourier Transform (cosine series)

Cross-sectional SLD provides internal sensitivity	Med-large Q-range
	Need low statistical unc.
	Prone to ringing



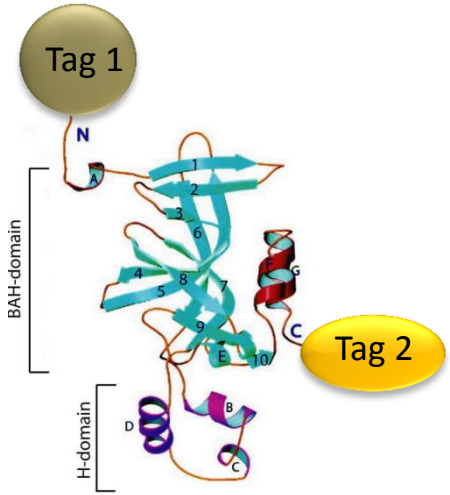
- Full SLD Inversion (over-determined set of equations, Gauss-Jordan elimination or single-value decomposition)

Maximum internal sensitivity	Sensitive to box-size binning
Q-range of 0.3 Å^{-1} → 1 nm resolution	Need low statistical unc.
3D analysis possible with appropriate tags	

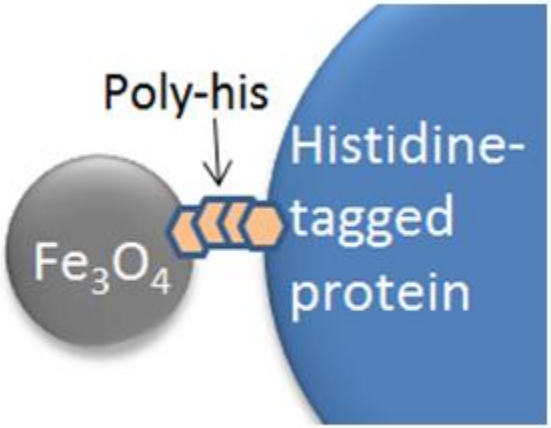


- <u>What other core-shell systems could benefit from this type of analysis</u> (Ca in casein, polymer, surfactant thickness)?

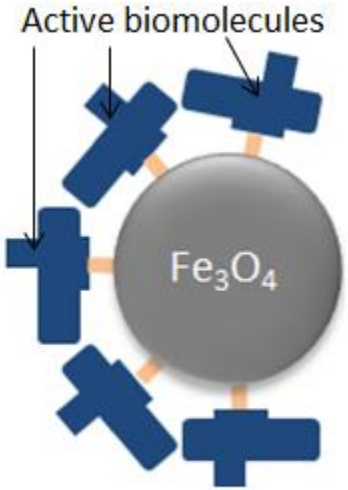
Anisotropic Tagging Ideas



Multiple-site tags



Site-specific Tagging

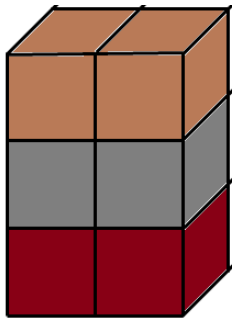


Many sites / tag

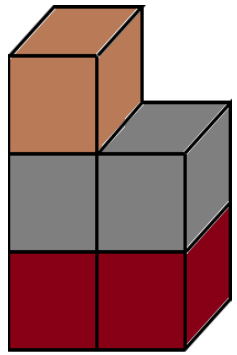
(Image from dissertation of Antje Geißenhöner, The role of the N-terminal acetyltransferase NatA in transcriptional silencing in *Saccharomyces cerevisiae*)

Nanowire Tagging

Anisotropic tags:

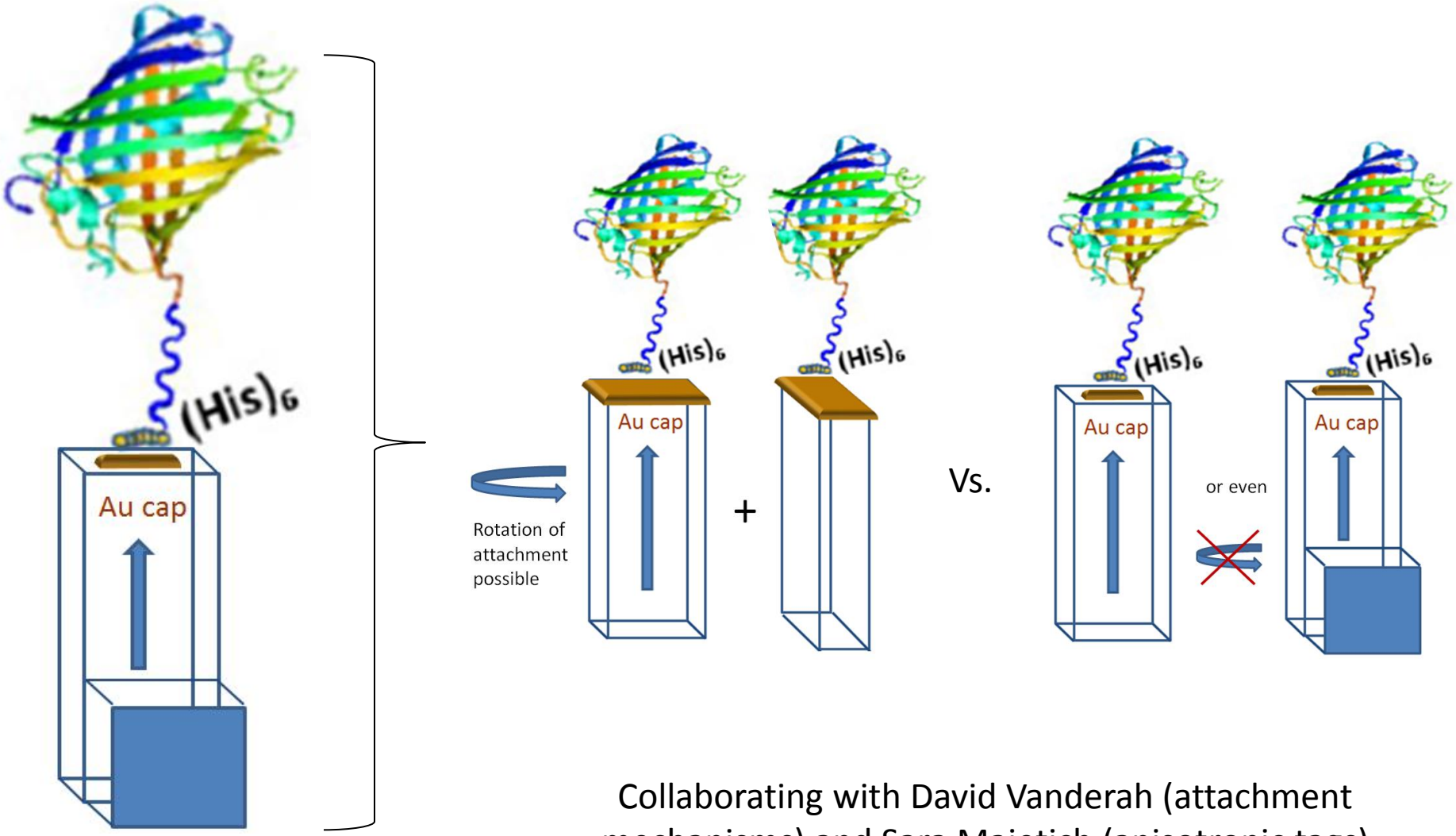


Rectangular tags



L-shaped tags

Idea for Oriented Anisotropic Tag Attachment



Collaborating with David Vanderah (attachment mechanisms) and Sara Majetich (anisotropic tags)

Thank you for your attention!

Questions?