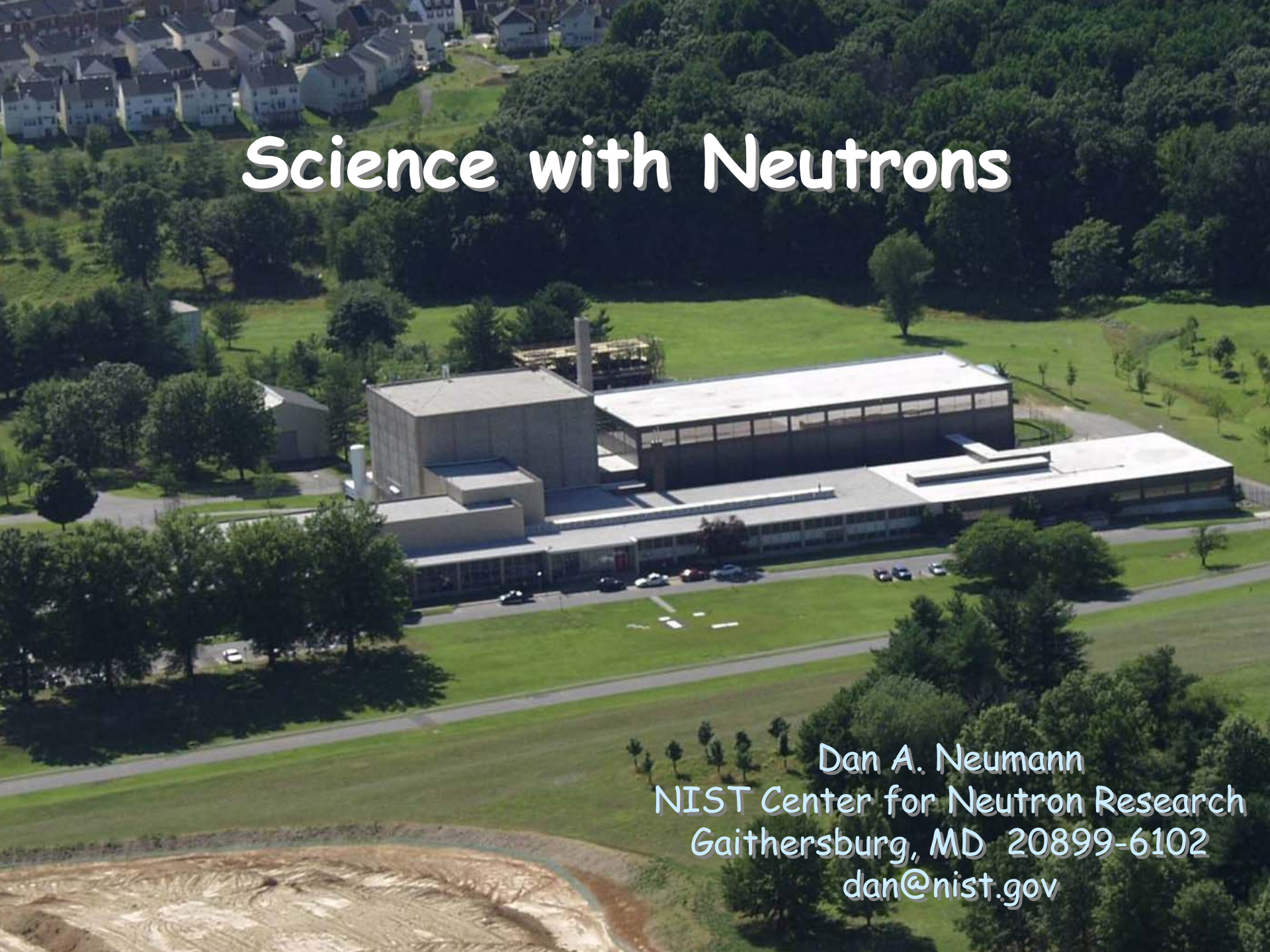
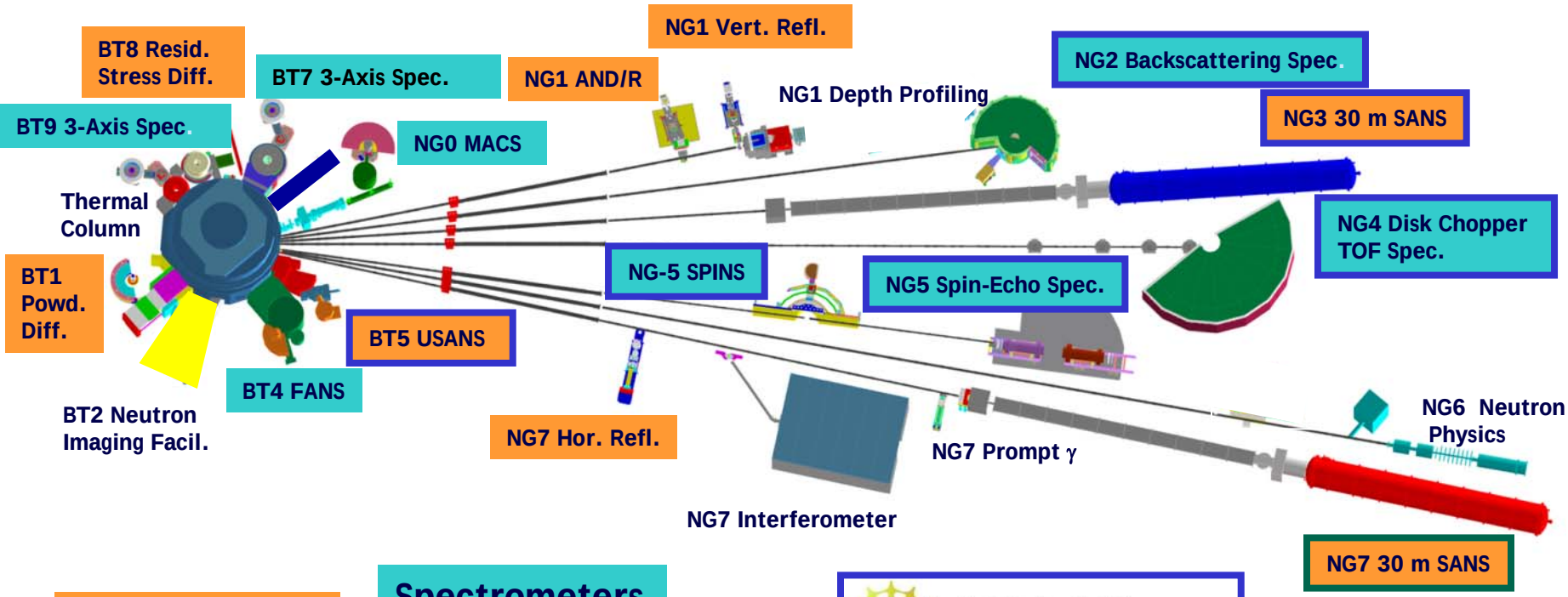
Science with Neutrons



Dan A. Neumann
NIST Center for Neutron Research
Gaithersburg, MD 20899-6102
dan@nist.gov

The NCNR Has 25 Operating Beam Instruments Tailored to Specific Needs …



Diffraction Instruments

Spectrometers

Other Neutron Methods

CHRNS Center for High Resolution Neutron Scattering NSF NIST

www.ncnr.nist.gov

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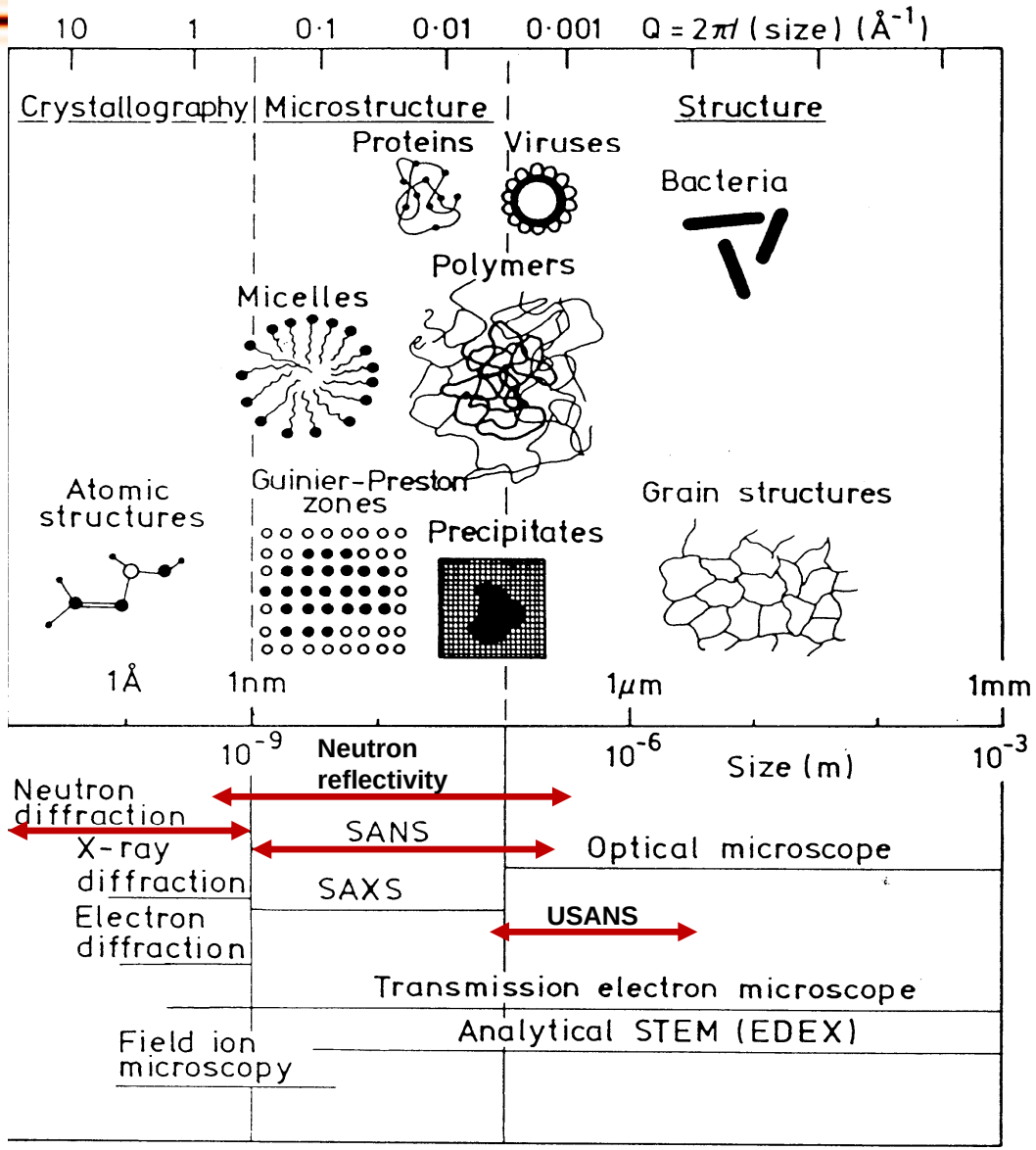
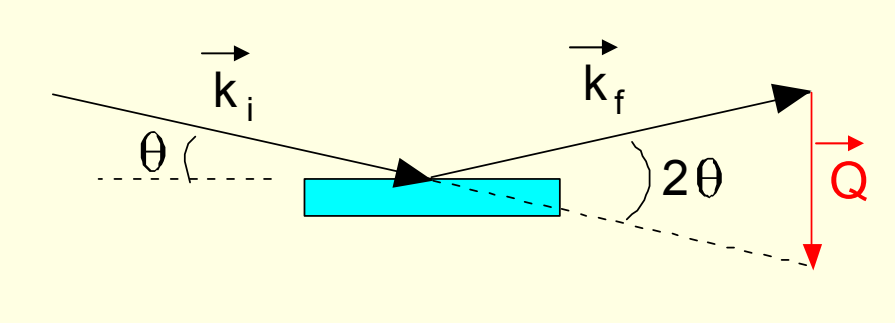
Techniques for the Measurement of Structure



Diffraction Probes Structure in the Direction of Q

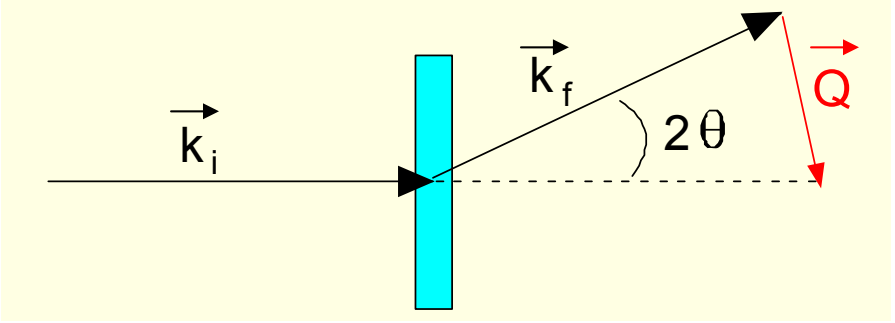
$$\vec{k}_i - \vec{k}_f = \vec{Q}$$

Specular Reflection Geometry



Reflectivity probes structure perpendicular to surface (parallel to Q), and *averages over structure in plane of sample*.

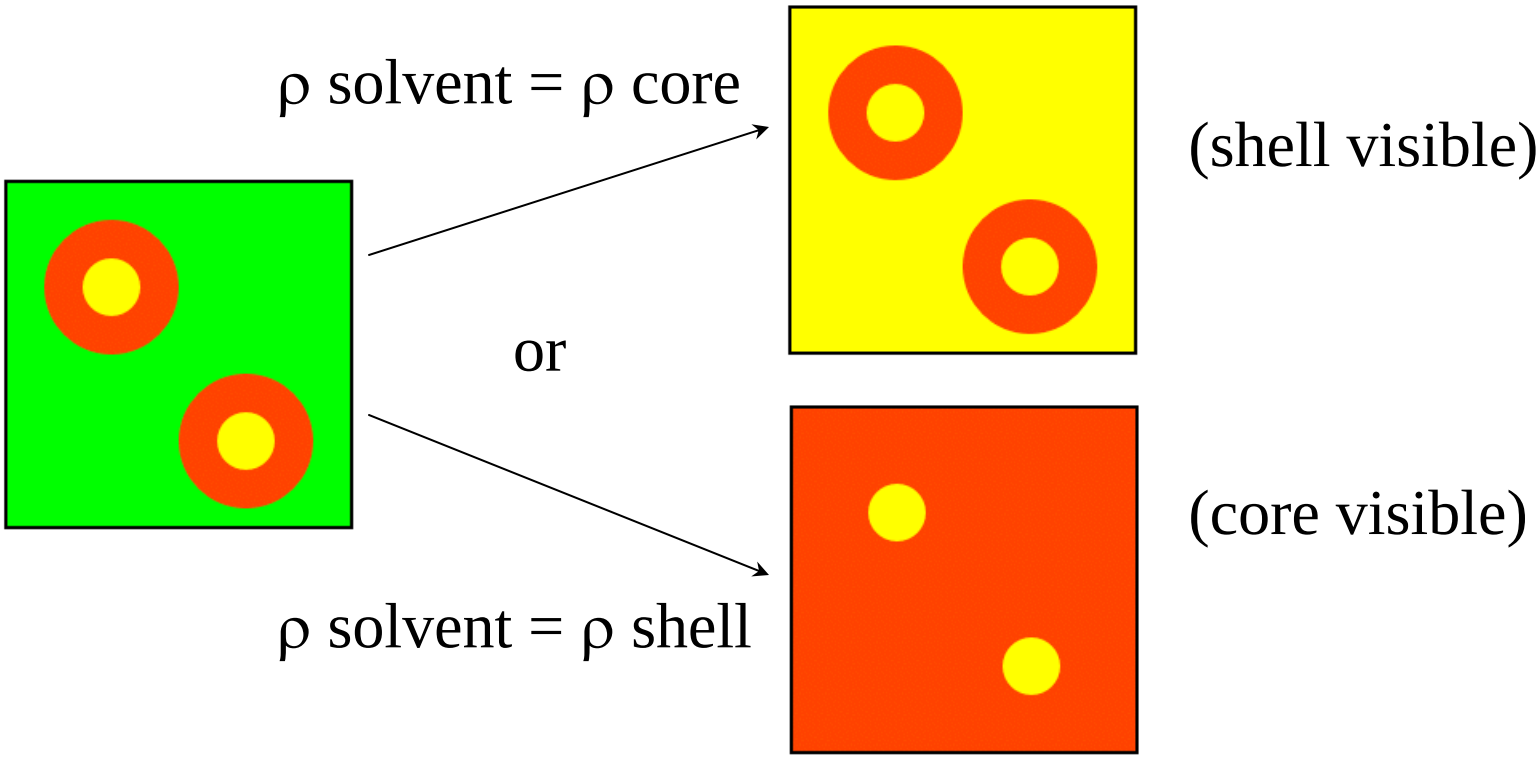
SANS Geometry



SANS probes structure in the plane (parallel to Q), and *averages over structure perpendicular to sample surface.*

Solving Multi-Phase Structures

Contrast Matching - reduce the number of phases "visible"



The two distinct 2-phase systems can be easily understood

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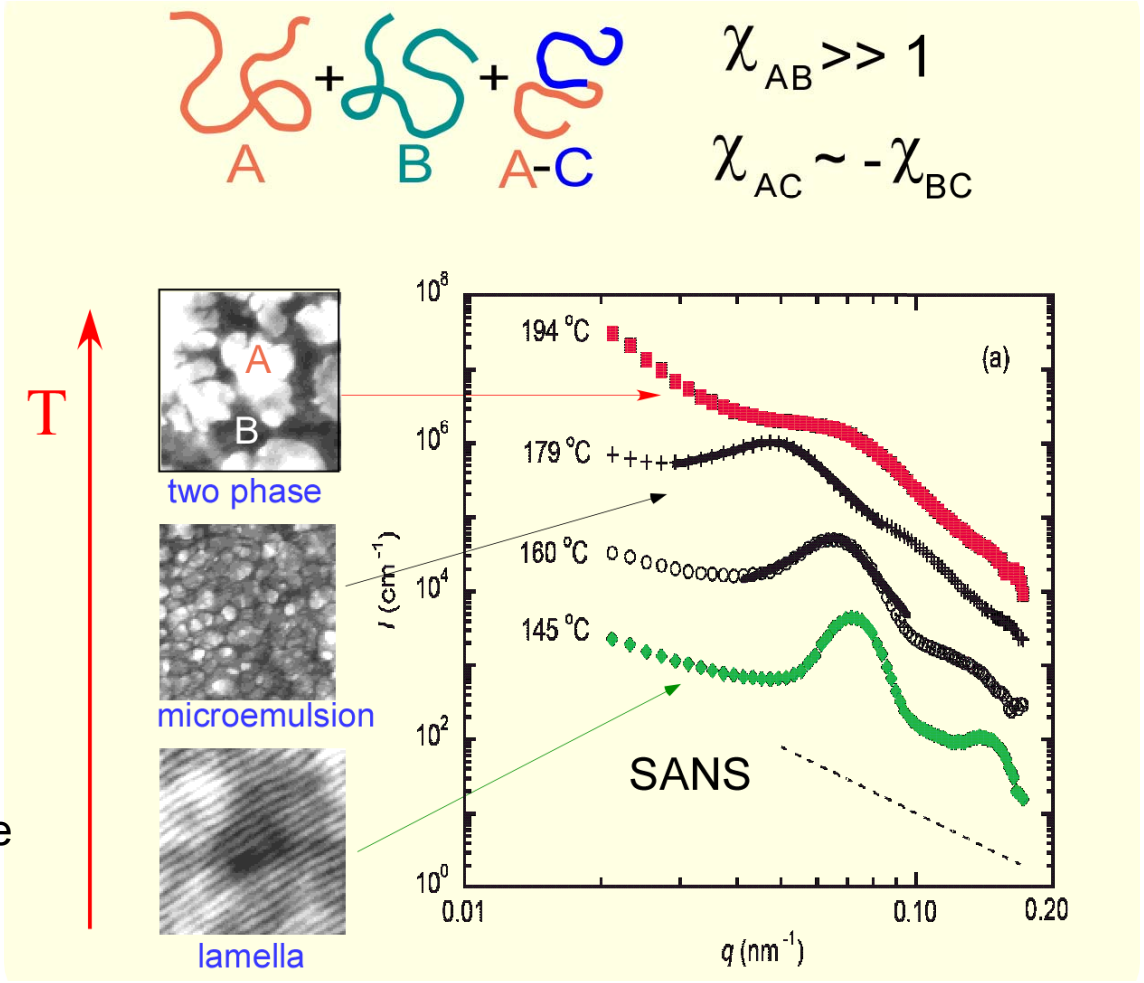
Polymers

All commercially important polymers are immiscible.

1) The blending of polymers to achieve desired properties is restricted.

2) The recycling of most commingled plastic waste is precluded.

One can select block copolymers that stabilize blends of even highly immiscible polymers by acting as a "surfactant". This is accomplished by choosing the block copolymer so that it balances the attractive and repulsive interactions between the copolymer and the A-rich and B-rich phases.

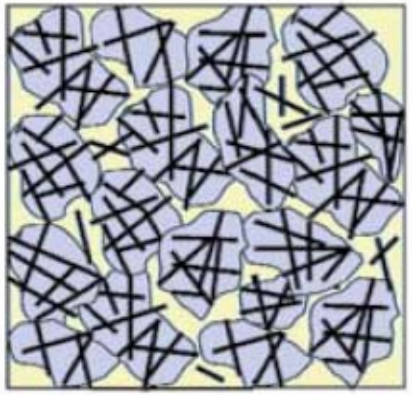


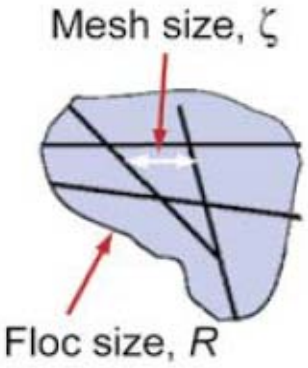
J.H. Lee *et al.*, Macromolecules **36**, 6537 (2003).

B.J. Reynolds *et al.*, Macromolecules **37**, 7401 (2004).

M.L. Ruegg *et al.*, Macromolecules **39**, 1125 (2006).

Polymer-SWNT nanocomposites



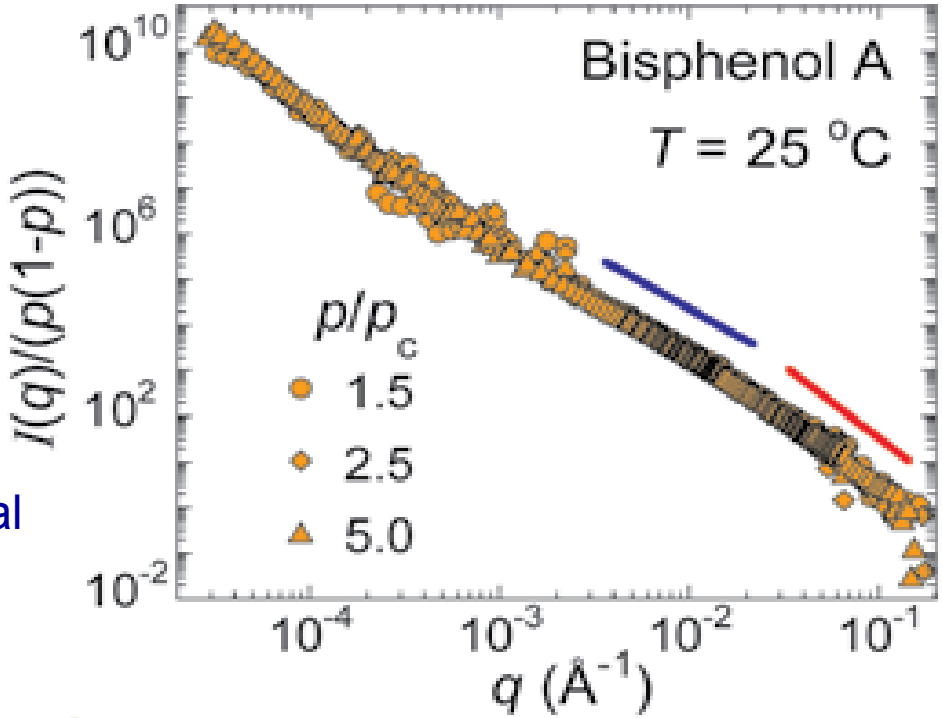


Network →Flocs (R)→ Mesh (ζ)→Single tube

R ≈ 4μm independent of concentration

SWNT's dispersed in polymer nanocomposites creates a percolated network structure above p_c

Scaling indicates a hierarchical network structure over a wide range of length scales



T Chatterjee, A. Jackson, R. Krishnamoorti, J. Am. Chem. Soc. **130**, 6934 (2008)

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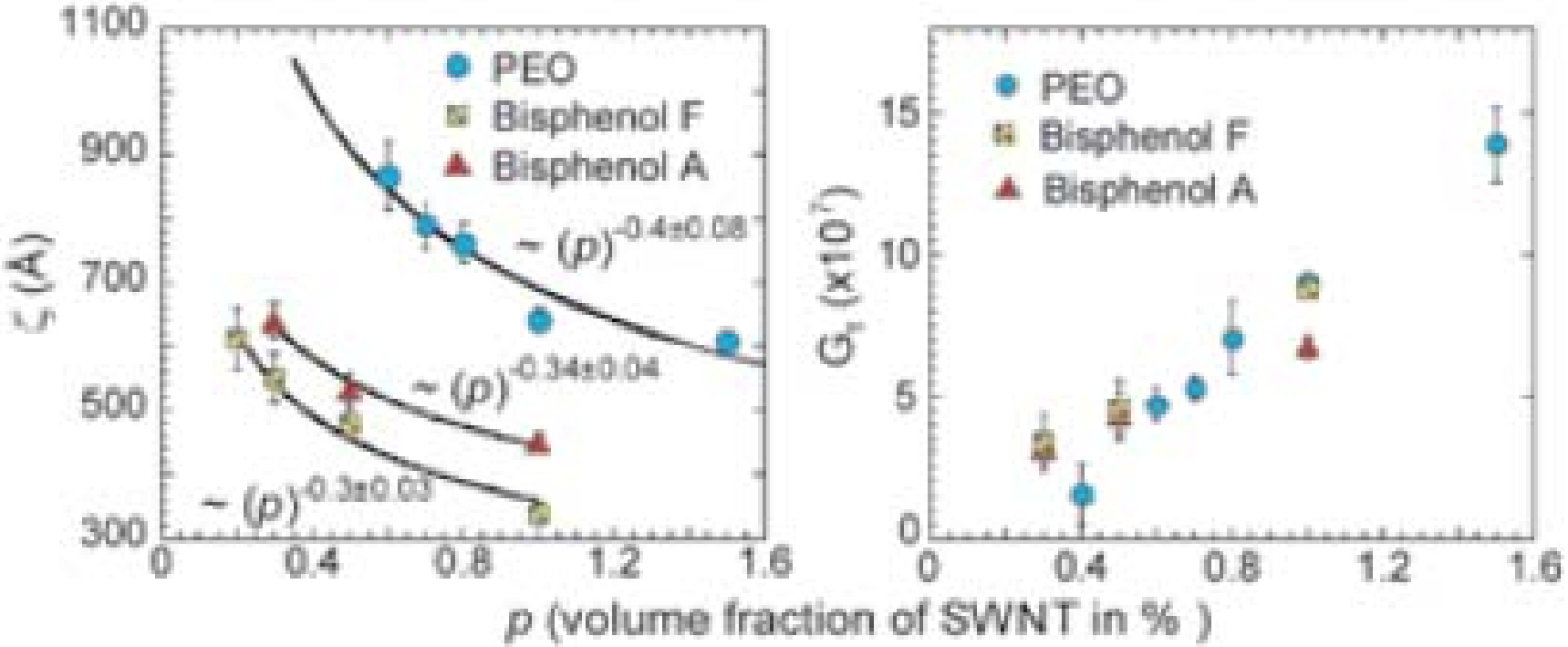
Polymer-SWNT nanocomposites



Weak mesh scaling can not explain the observed scaling exponent

The interactions between flocs (either directly or mediated by polymer), control the scaling dependence of the elastic strength of the network

T Chatterjee, A. Jackson, R. Krishnamoorti, J. Am. Chem. Soc. **130**, 6934 (2008)

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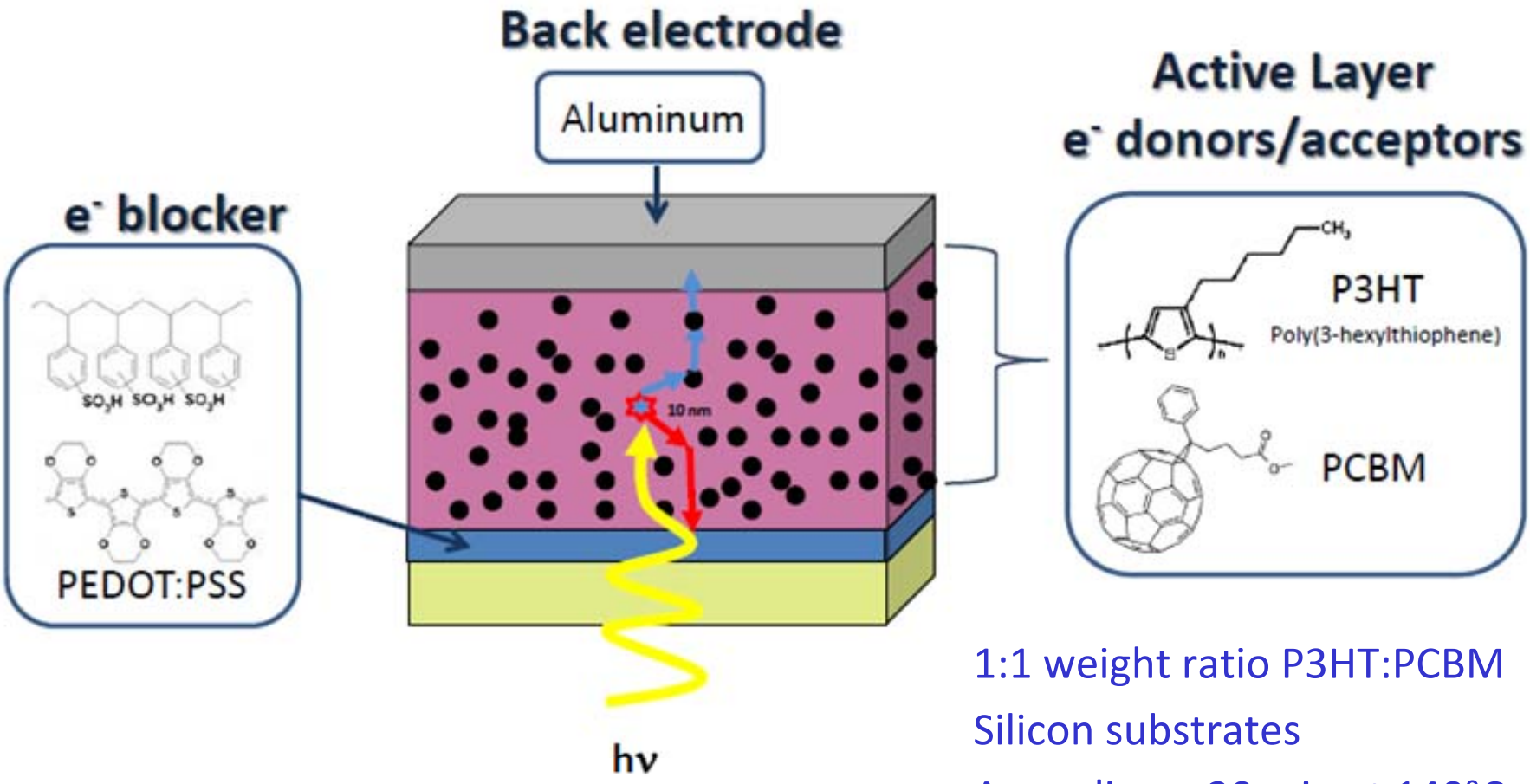
Organic Solar Cells



1:1 weight ratio P3HT:PCBM

Silicon substrates

Annealing - 20 min at 140°C

J. Kiel, B.J. Kirby, C. Majkrzak, B. Maranville, and M. Mackay, submitted.

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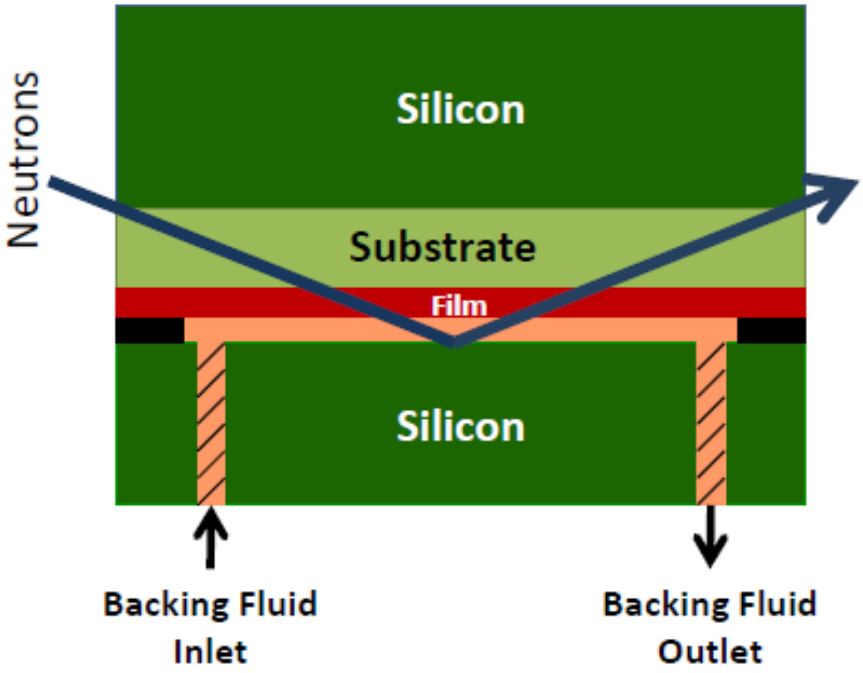
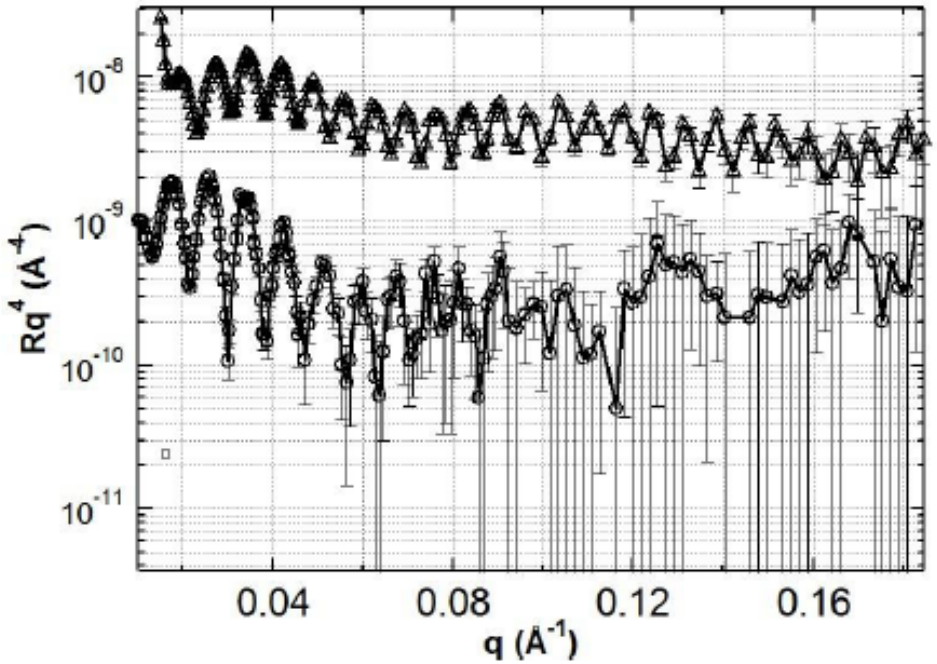
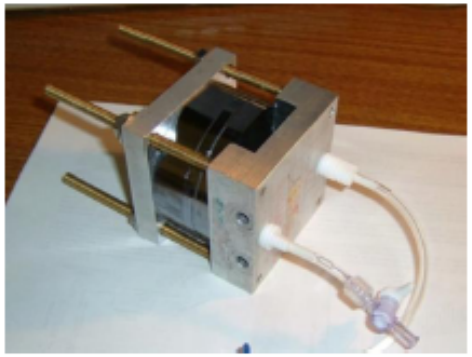
Neutron Reflectivity



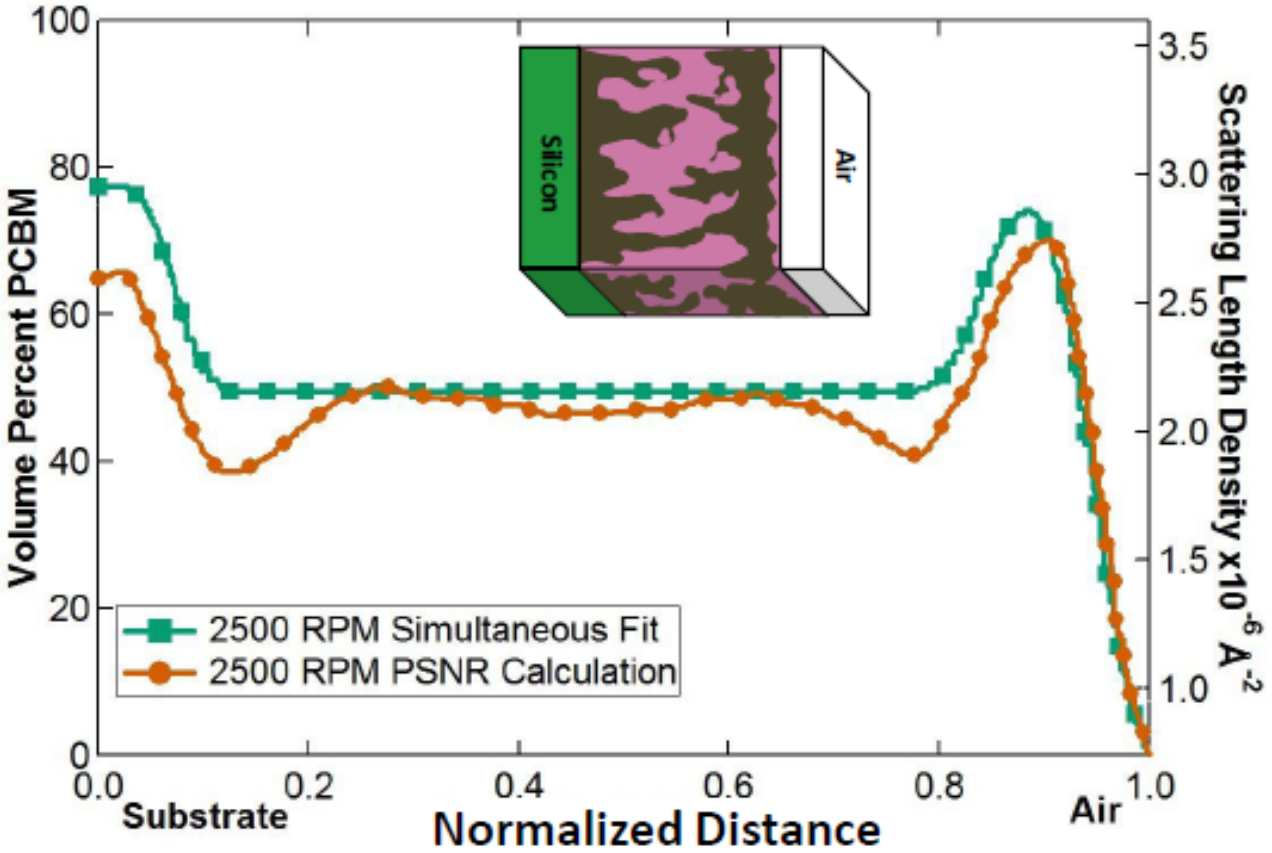


Addition of high SLD backing media greatly enhances scattering intensity and statistics



J. Kiel, B.J. Kirby, C. Majkrzak, B. Maranville, and M. Mackay, submitted.

Dispersion of PCBM



- Simultaneous fitting and PSNR calculations show agreement
- High PCBM concentration at substrate
- High PCBM concentration near air interface

J. Kiel, B.J. Kirby, C. Majkrzak, B. Maranville, and M. Mackay, submitted.

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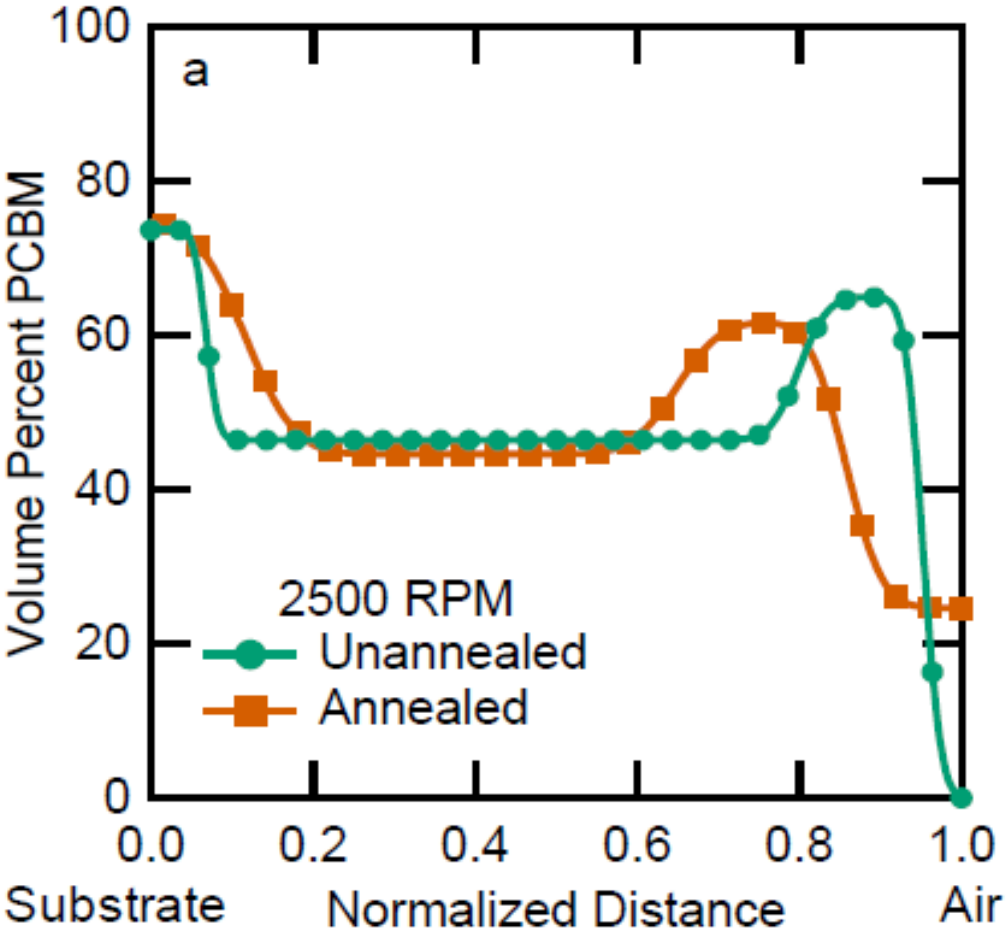
Effect of Annealing



- Silicon substrate with 40 nm PEDOT:PSS
- Annealed 140°C for 20 minutes
- PCBM concentration increases from 0.2% to 25% at air interface
- Energy conversion efficiency increases by a factor of 4

J. Kiel, B.J. Kirby, C. Majkrzak, B. Maranville, and M. Mackay, submitted.

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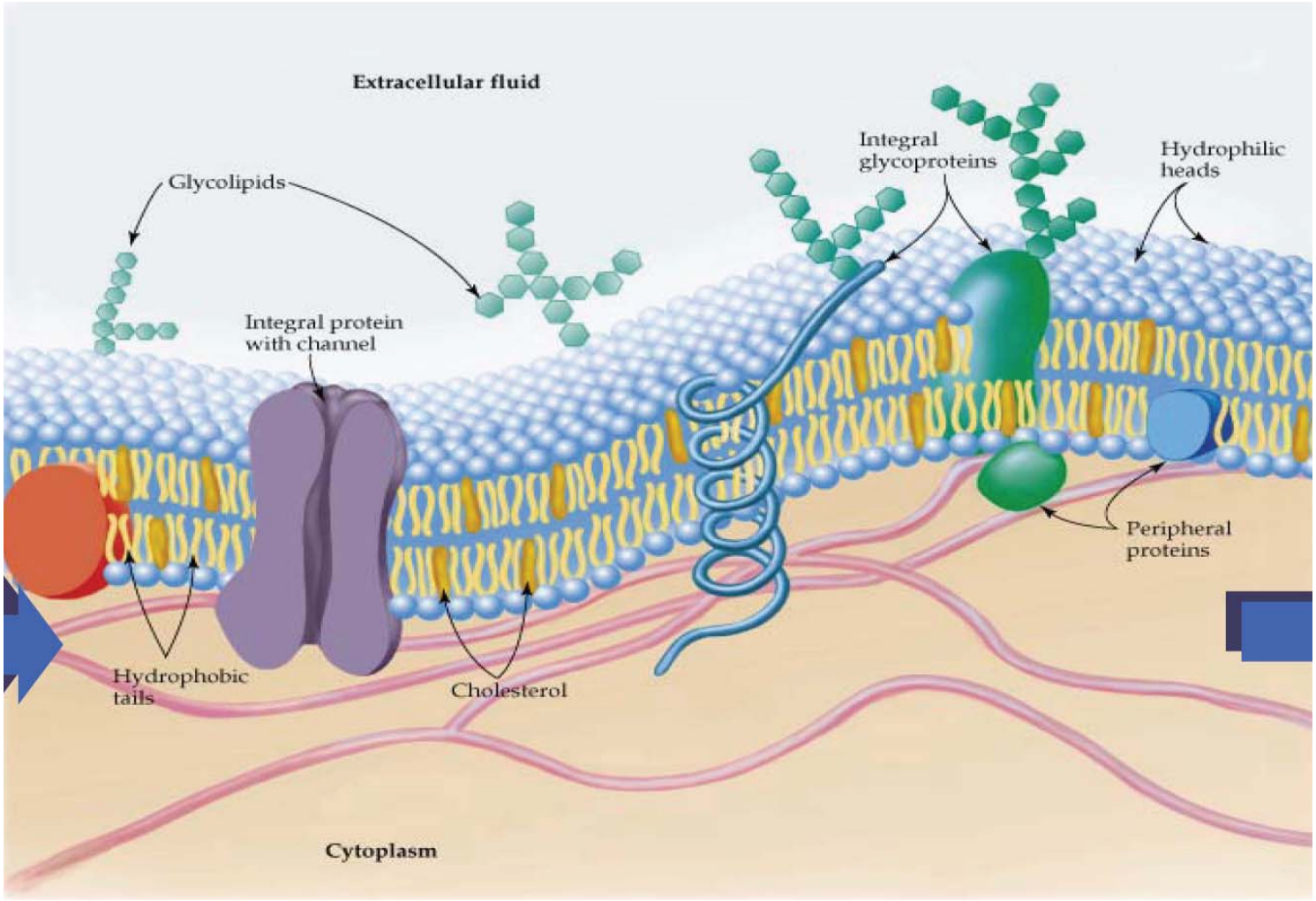
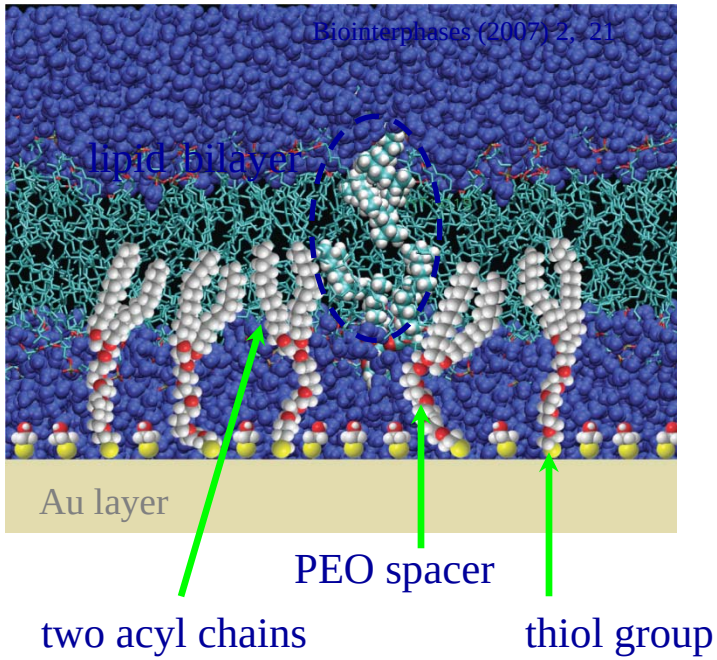
Phospholipid Membranes



Tethered Bilayer Membranes (tBLM)

Bio-mimetic environment for studying protein-lipid interactions
(developed at NIST)



- Tether partially decouples bilayer from substrate
- Accommodate Proteins with sub-membrane domains
- Fluid bilayer is highly stable
  - Data acquisition times of several days
  - Resilient to exchange of aqueous phase
  - In situ sample manipulation

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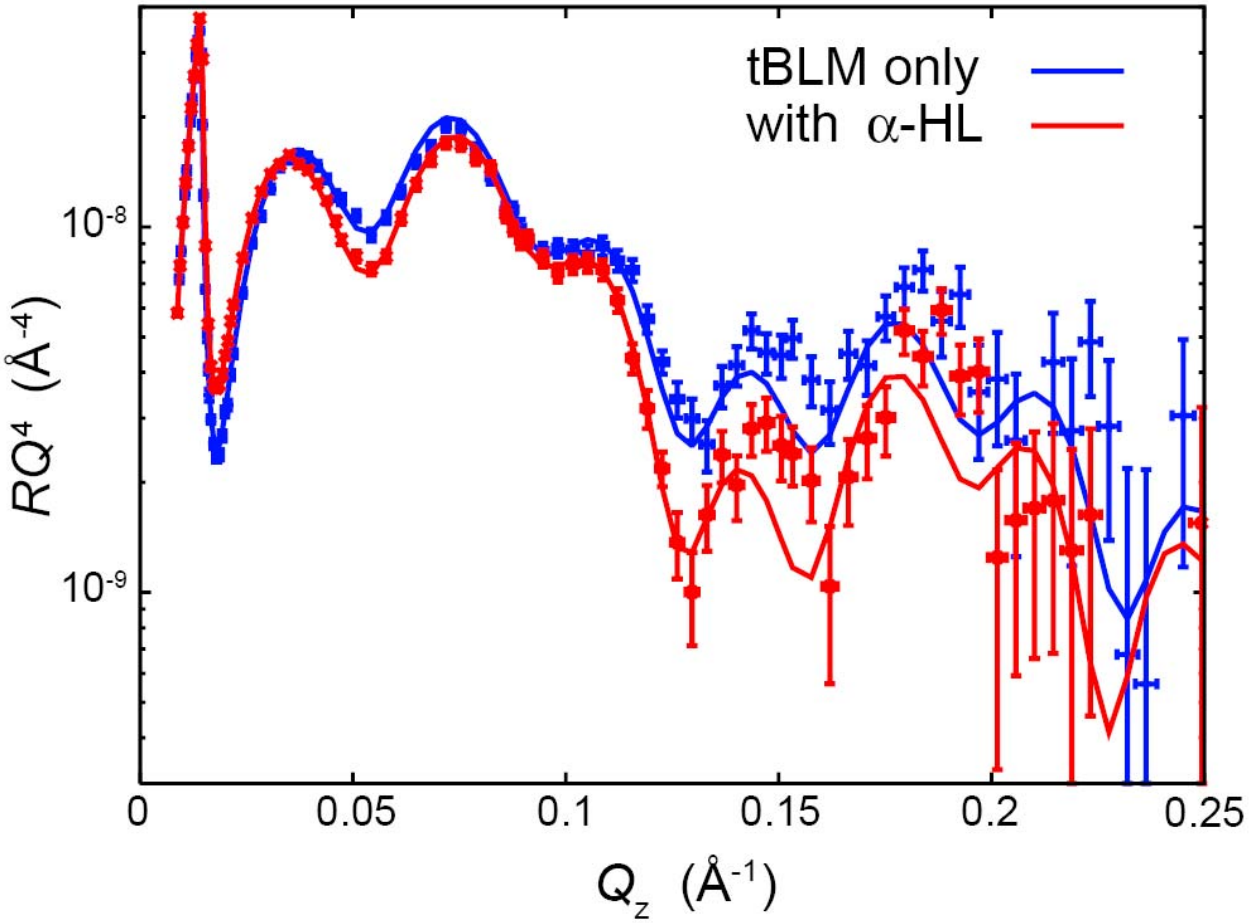
α-hemolysin in a Biomimetic Membrane



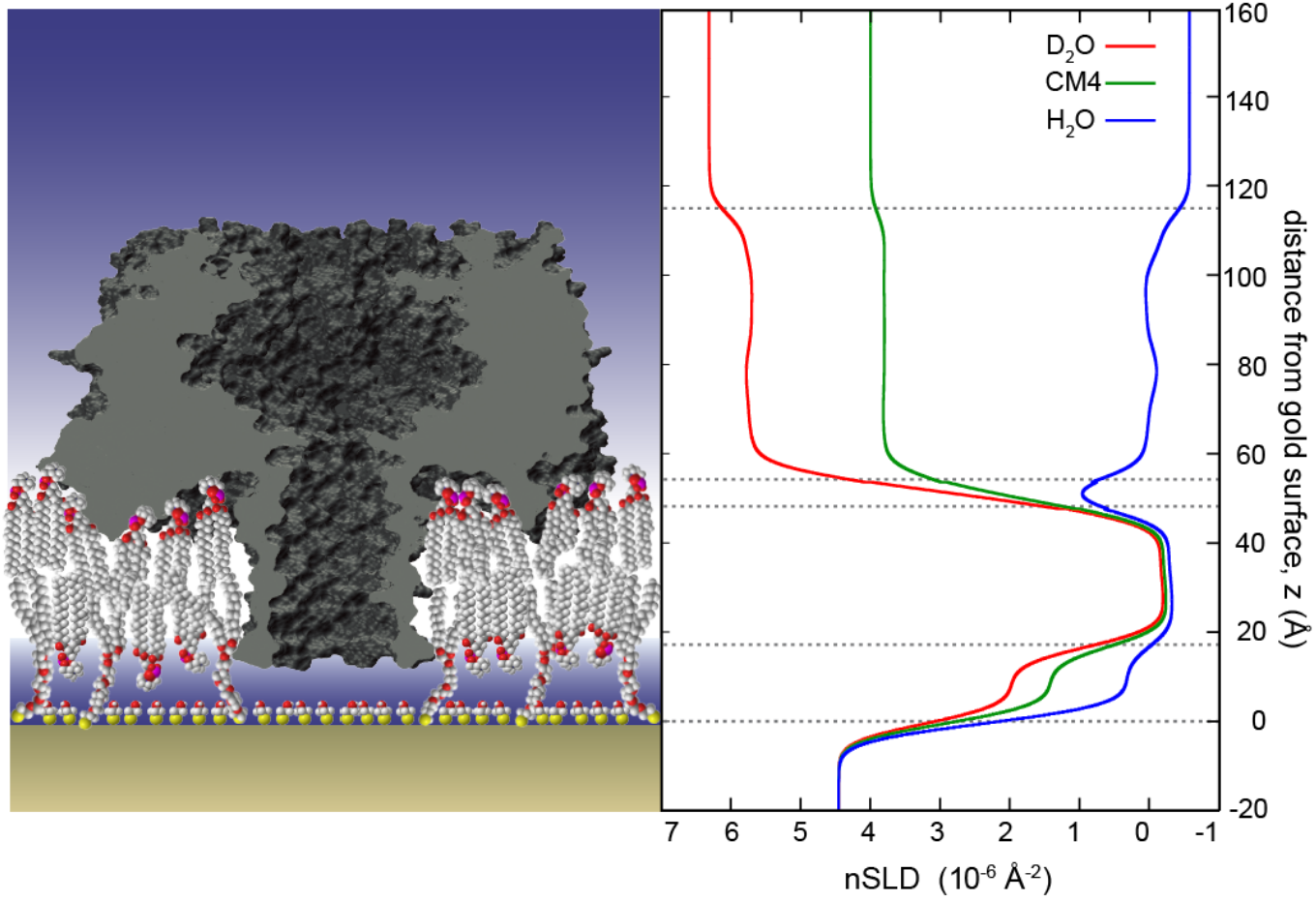
Toxins sometimes kill cells by forming pores in the cell membrane.

α-hemolysin (αHL) is a toxin produced by *Staphylococcus aureus.*

D.J. McGillivray, F. Heinrich, M. Lösche, I. Ignatjev G. Valincius, D.J. Vanderah, and J.J. Kasianowicz, Biophys. J. **96**, 1547 (2009).

NIST

α-hemolysin in a Biomimetic Membrane



The protein rim is seen to interact strongly with the lipid headgroups.

The crystal structure of the toxin was used in the fits.

D.J. McGillivray, F. Heinrich, M. Lösche, I. Ignatjev
G. Valincius, D.J. Vanderah, and J.J. Kasianowicz,
Biophys. J. **96**, 1547 (2009).

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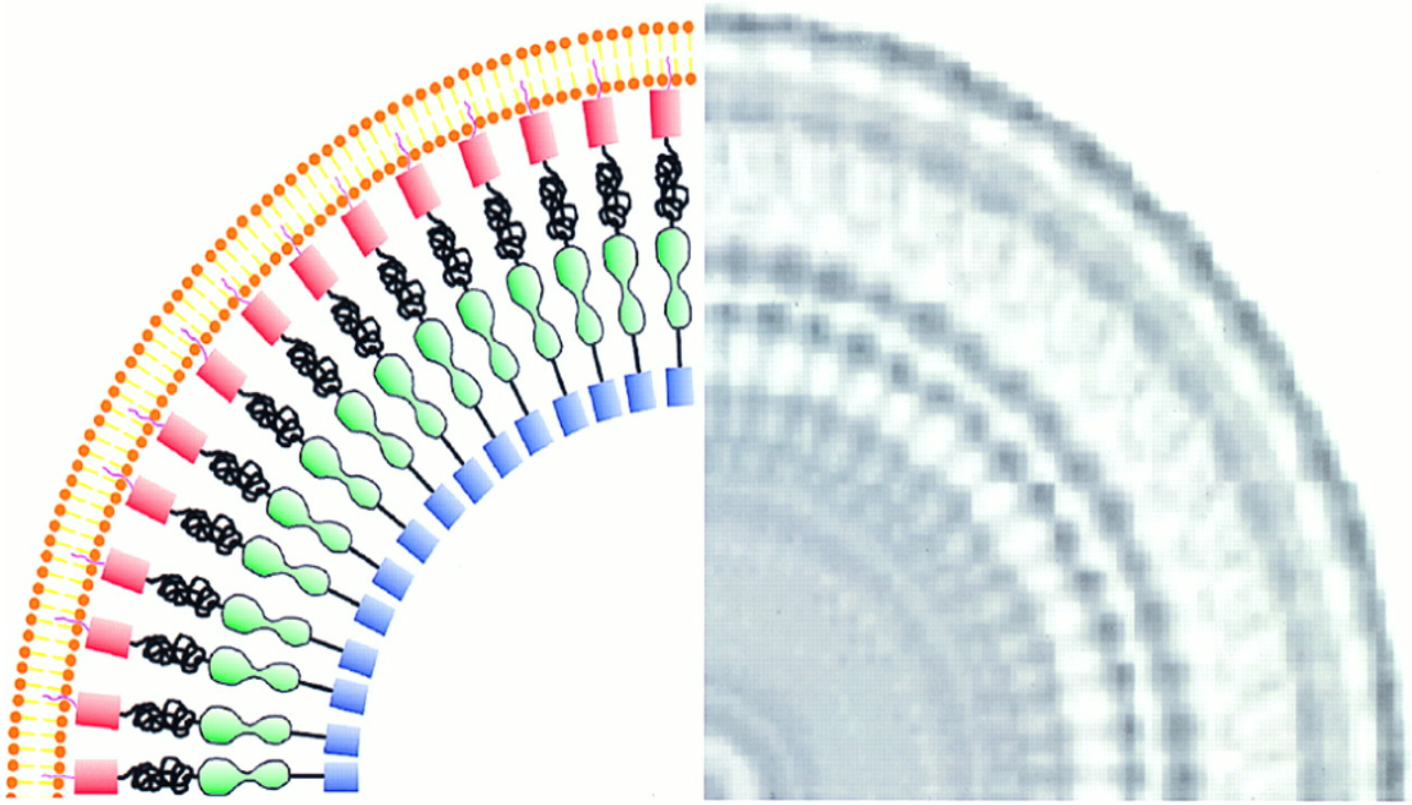
Basic Structure of an Immature Retrovirus

Biochemical evidence suggests that HIV-1 Gag is NOT extended in solution.



Yeager et al., PNAS 95: 7299, 1998

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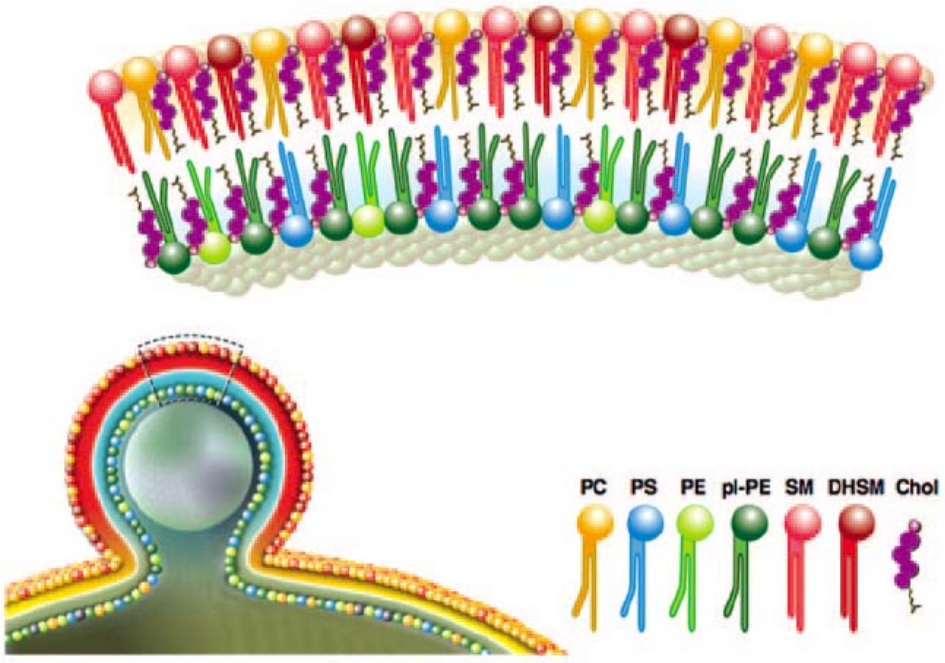
Mimicking the Viral Lipidome



Lipid bilayer composition chosen to mimic viral lipidome:

- d_{54} -DMPC (d-DMPC, zwitterionic)
- DMPS (anionic, increases electrostatic interactions
- Cholesterol

d-DMPC:DMPS:Cholesterol = 70:30:3 produced the most complete bilayer

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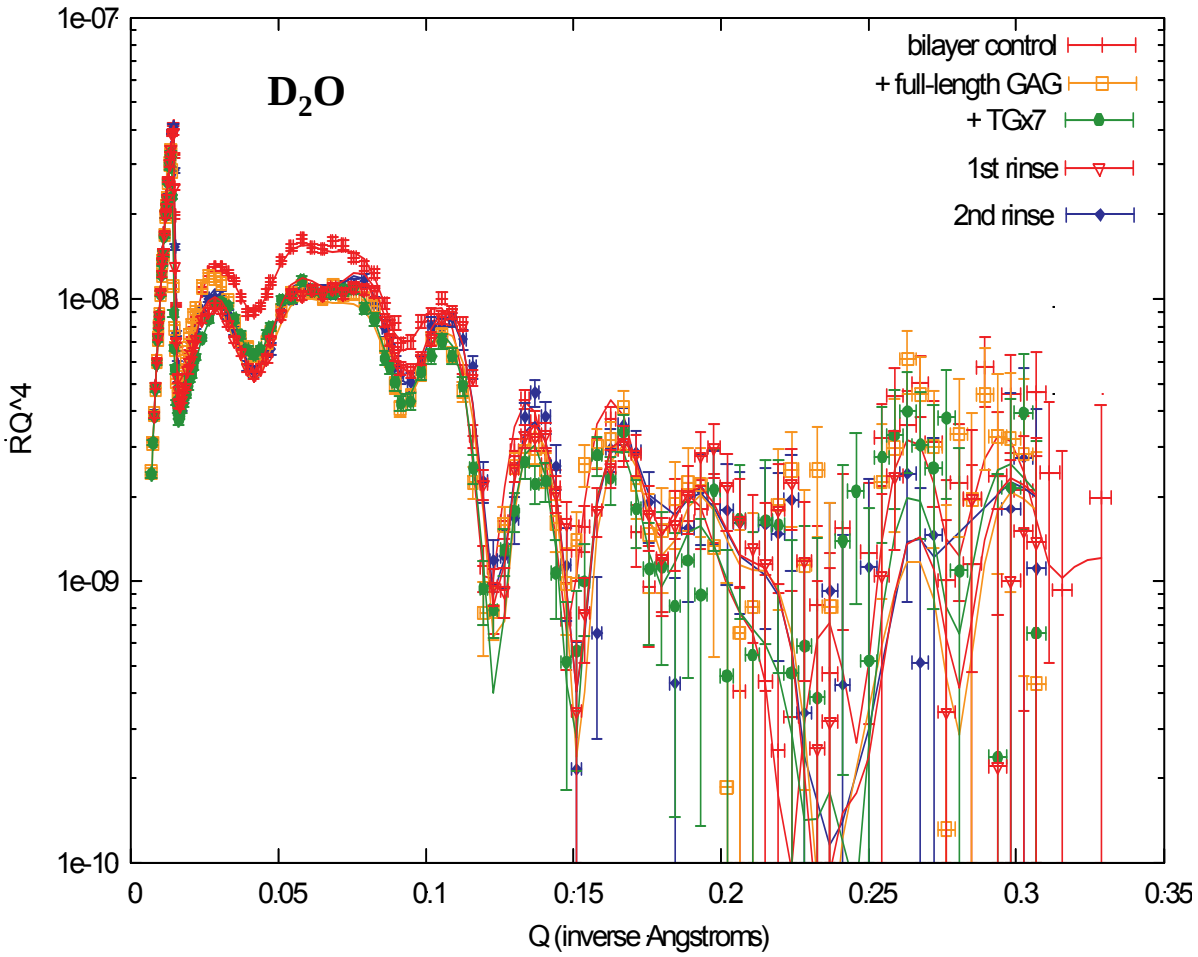
Modeling the Gag Protein Layer



SLD profiles determined by simultaneous fitting of **13** measurements:

- Three contrasts (D_2O, H_2O and CM4) for
- Bilayer control
- Gag Binding
- Gag + TG14 DNA
- Rinse 1: 250 mM NaCl

- Rinse 2: 500 mM NaCl only measured in D_2O

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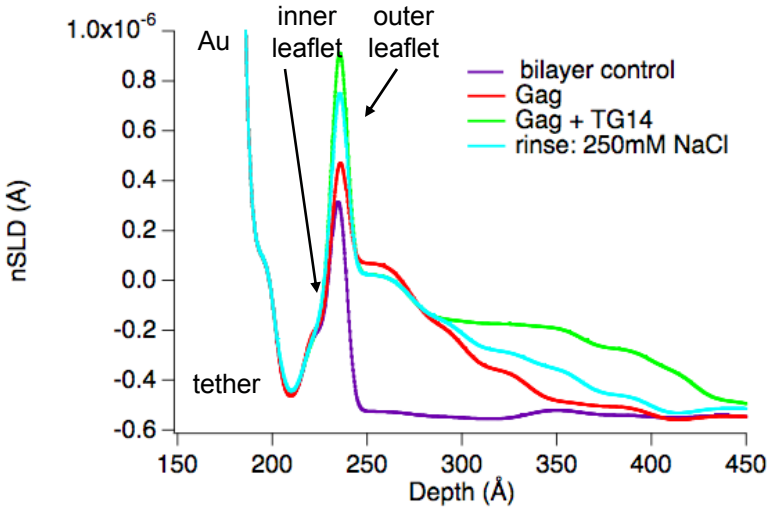
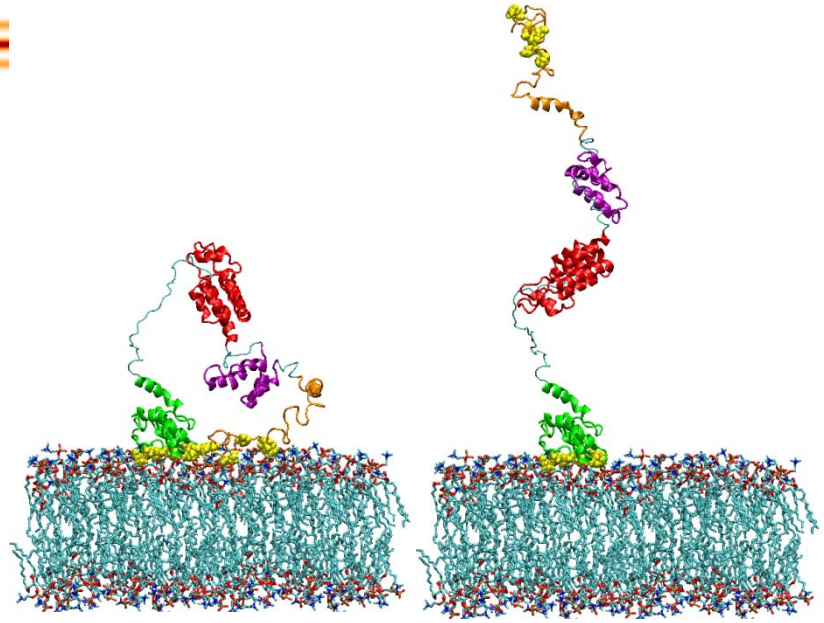
Gag Layer On Membrane Surface





nSLD increases for distances beyond the lipid bilayer surface.

nSLD increases at greater distances from the lipid bilayer surface.

High salt rinse removes DNA and original profile is recovered.

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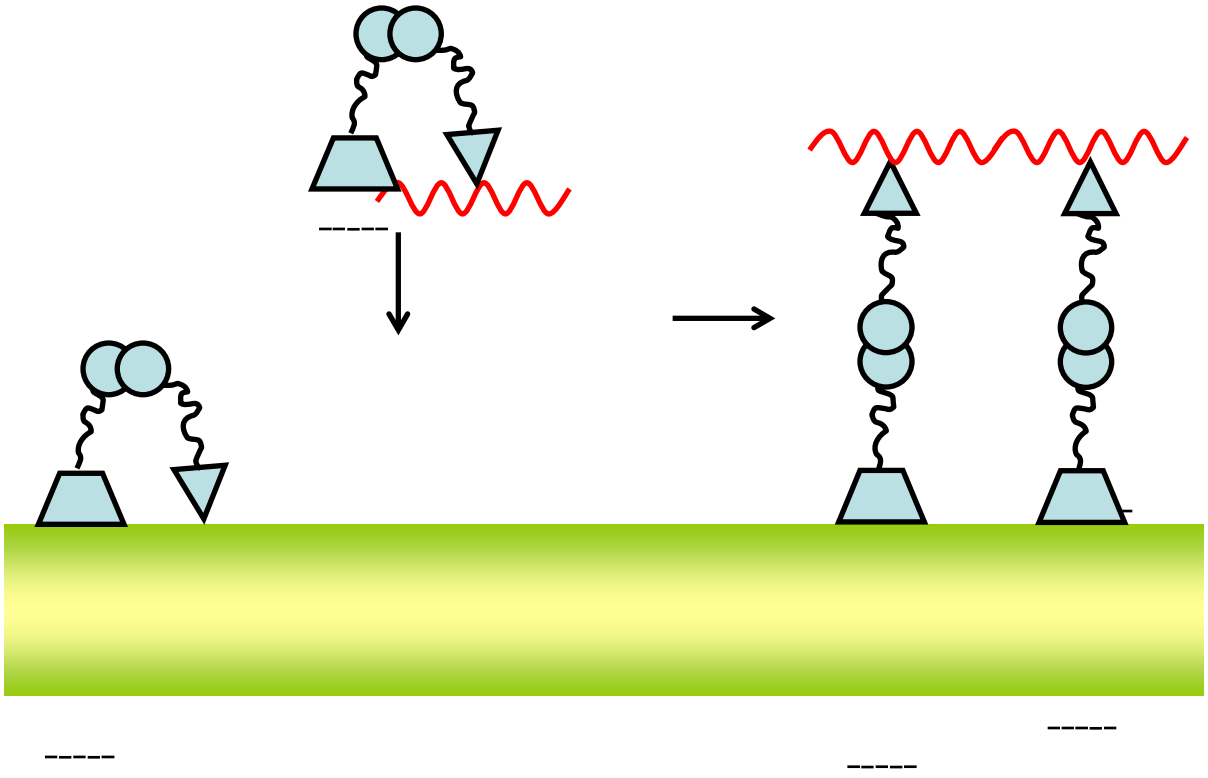
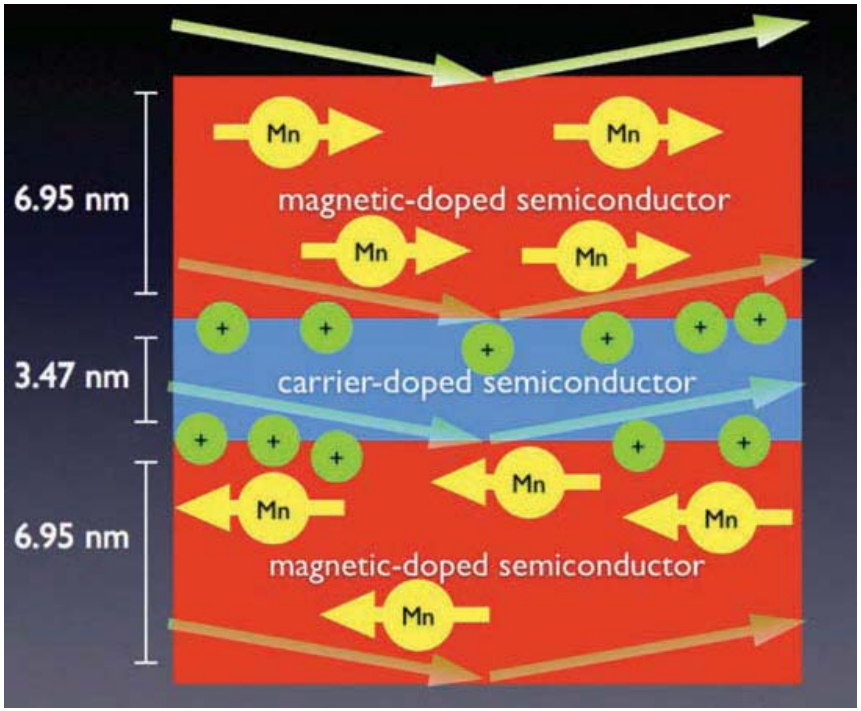
Model for Gag Assembly on Bilayer

Both nucleic acid and lipid binding
are needed for extension of Gag protein



Magnetic Semiconductors - Spintonics



Ferromagnetic coupling is typically observed

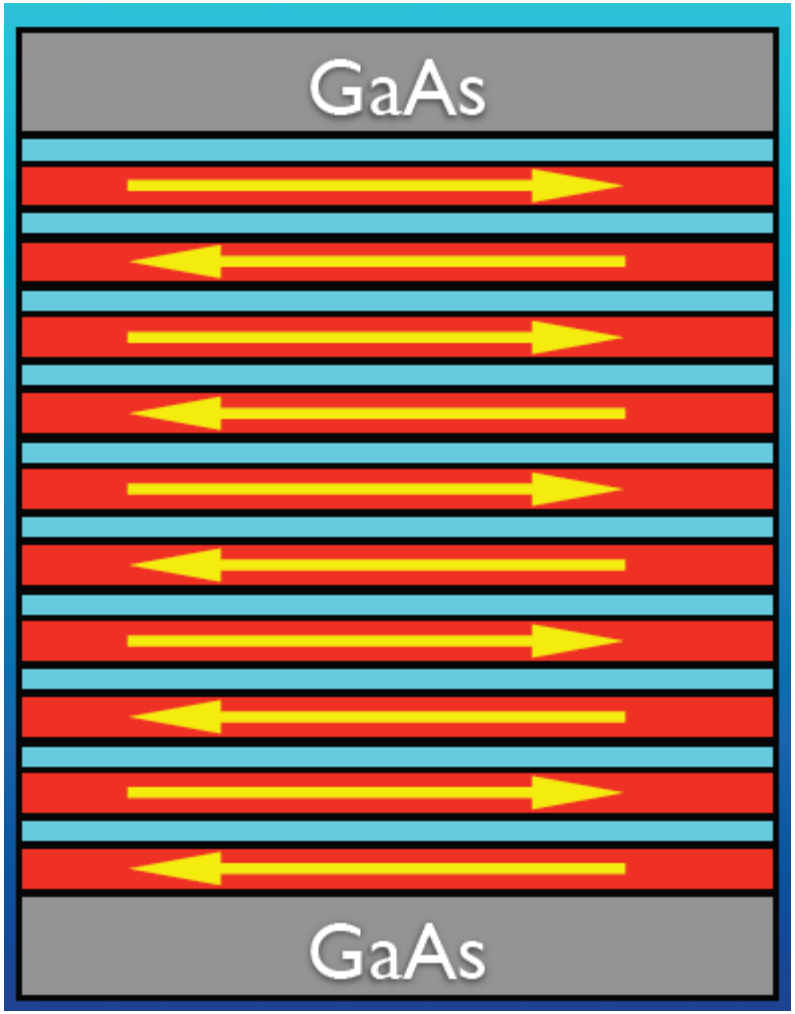
Would like antiferromagnetic coupling
- device applications
- understand exchange $\uparrow T_c$

10 layers 6.95 nm $Ga_{0.97}Mn_{0.03}As$ separated by 3.47 nm GaAs:Be (10^{20} cm^{-3} hole doping)

Also a sample with no Be

NIST

Magnetic Semiconductors - Spintonics



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Also a sample with no Be

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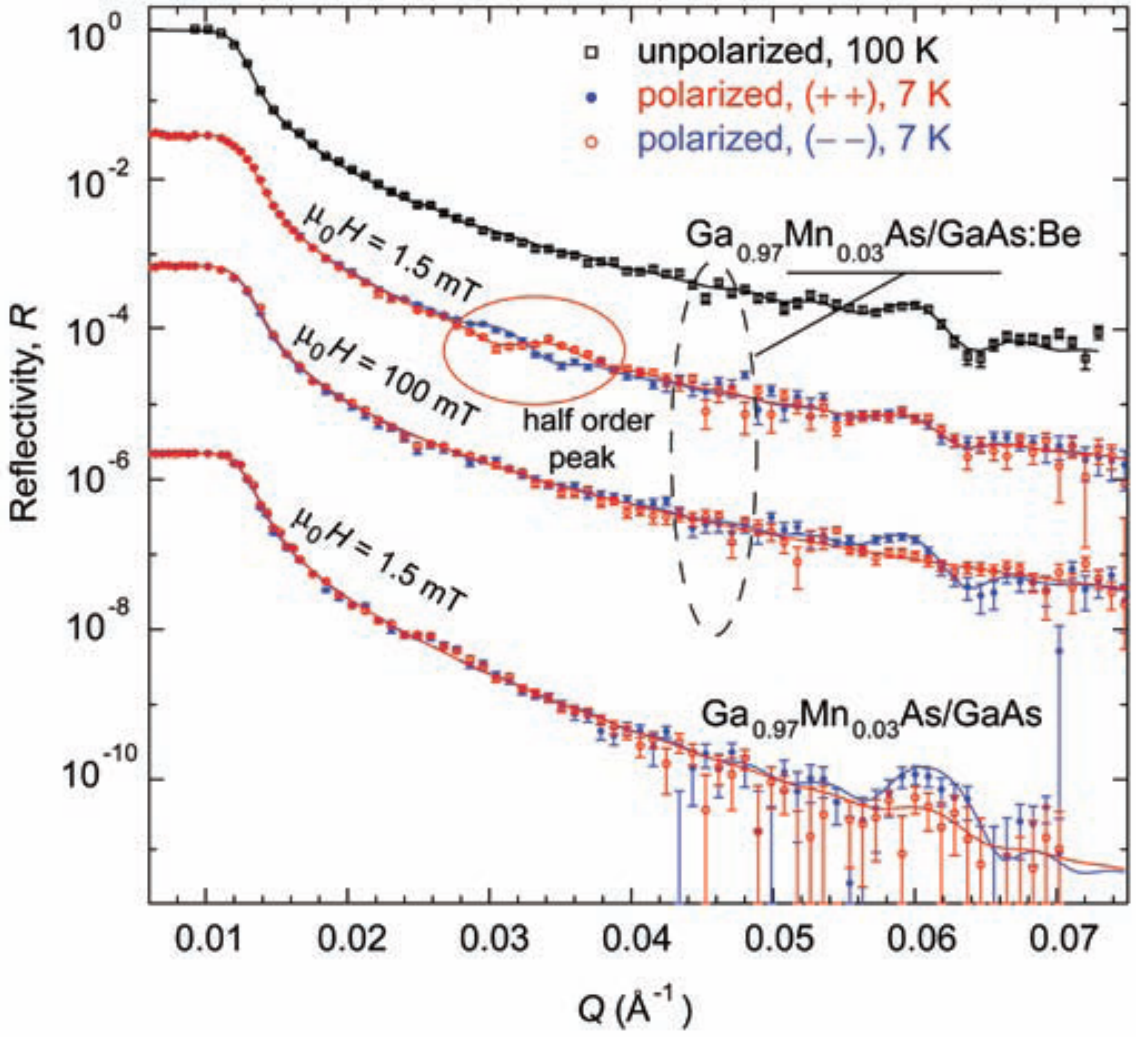
Polarized Neutron Reflectometry Reveals AF Coupling



J.-H. Chung *et al.*, PRL **101**, 237202 (2008).

Specular Reflectivity

1st order Bragg Peak (10.4 nm)

At 7K – applied 1.5 mT field
- Polarization dependent
- ½ order peak appears

⇒Antiferromagnetic coupling

Apply 100 mT
- ½ order peak disappears

Undoped spacer
- No ½ order peak

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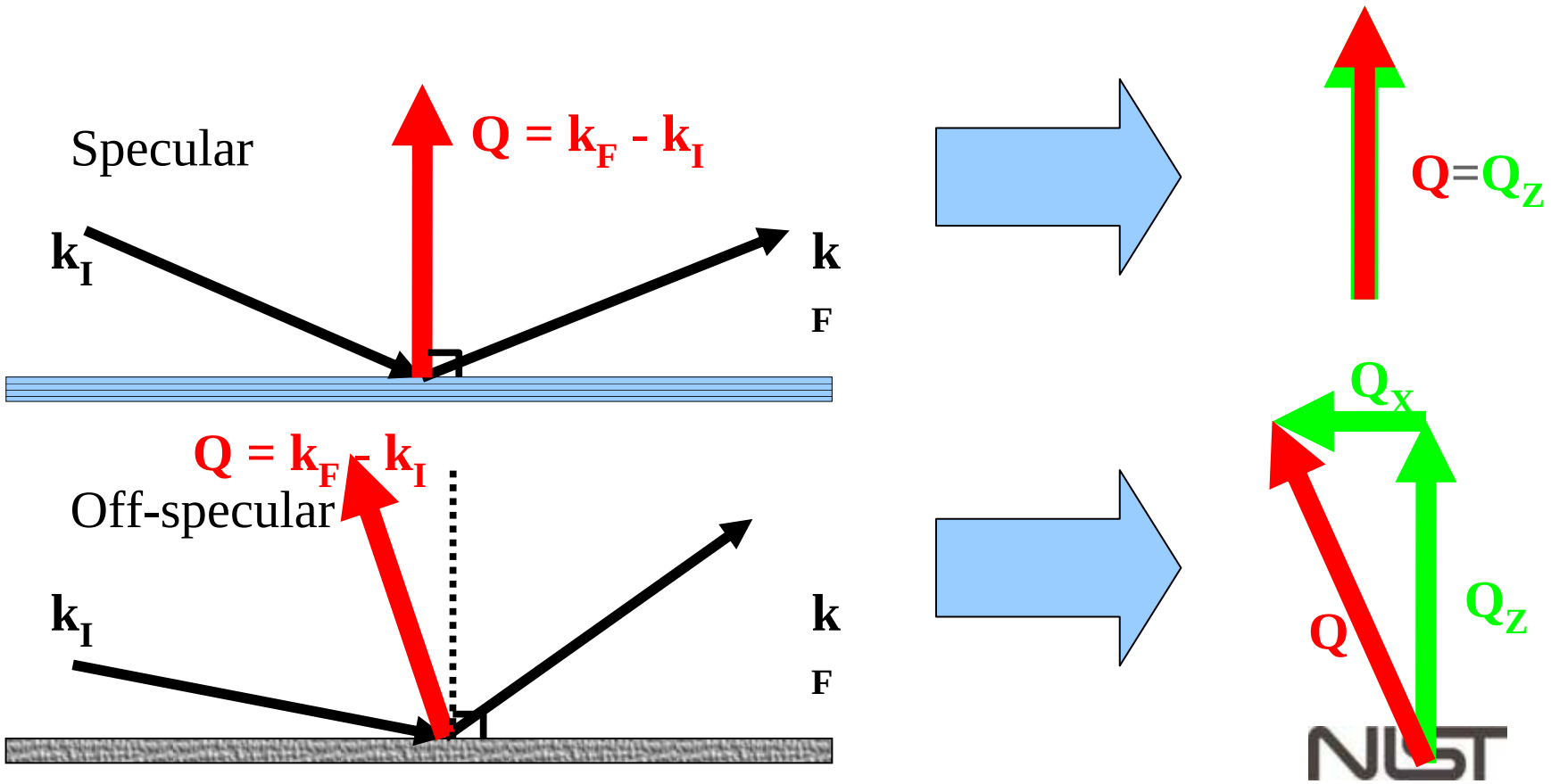
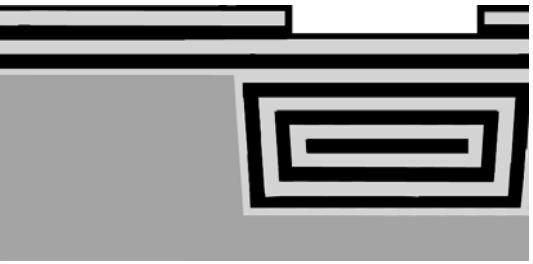
Off-specular neutron reflectometry

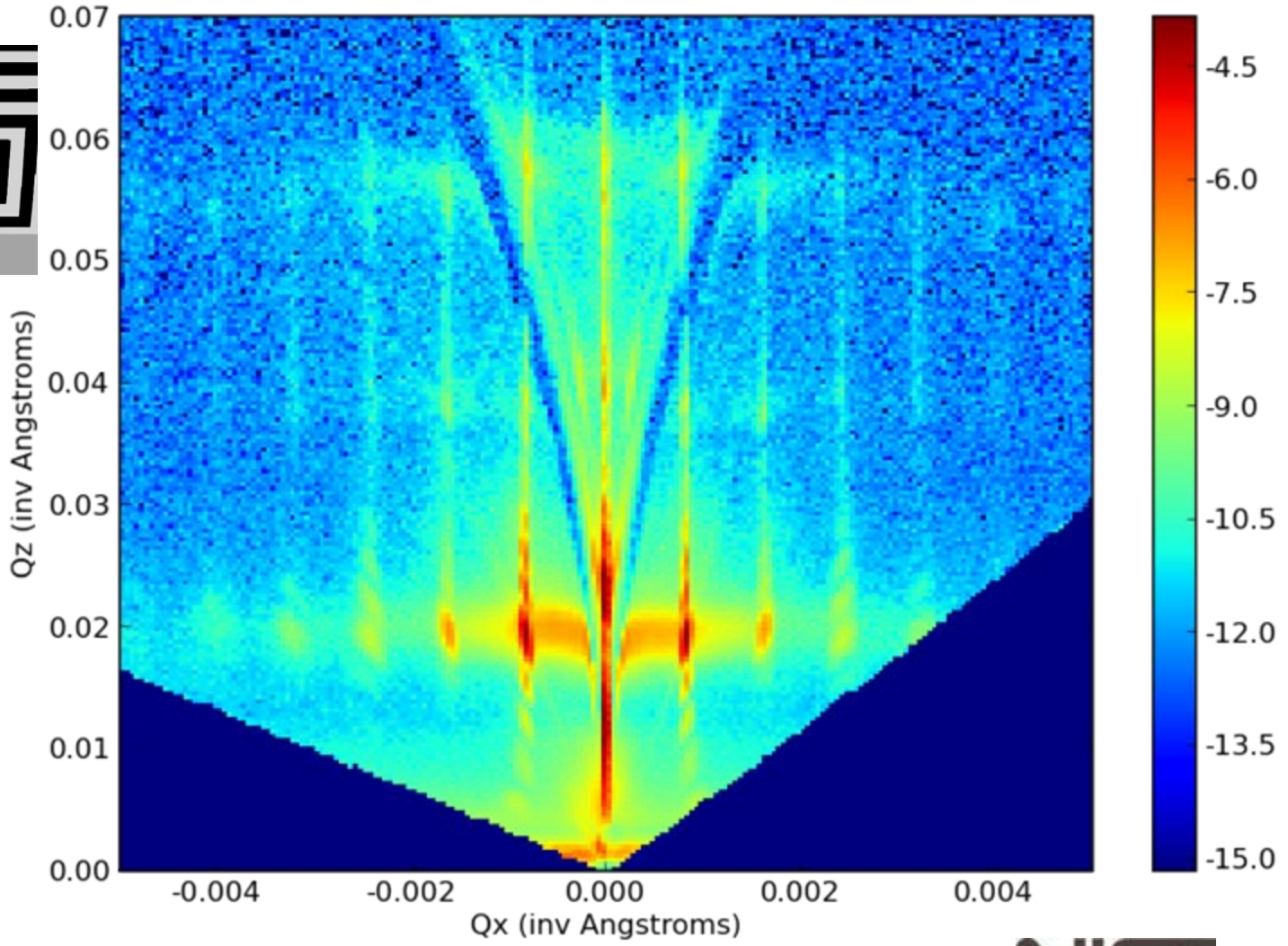
For patterned films

- probes length scales larger than SANS



Block Co-polymer in a Si Grating





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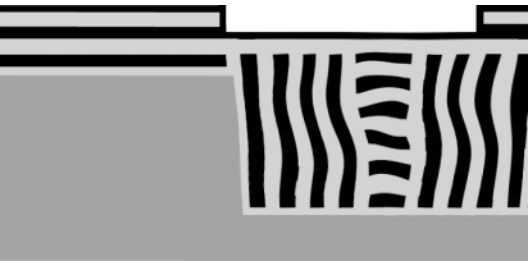
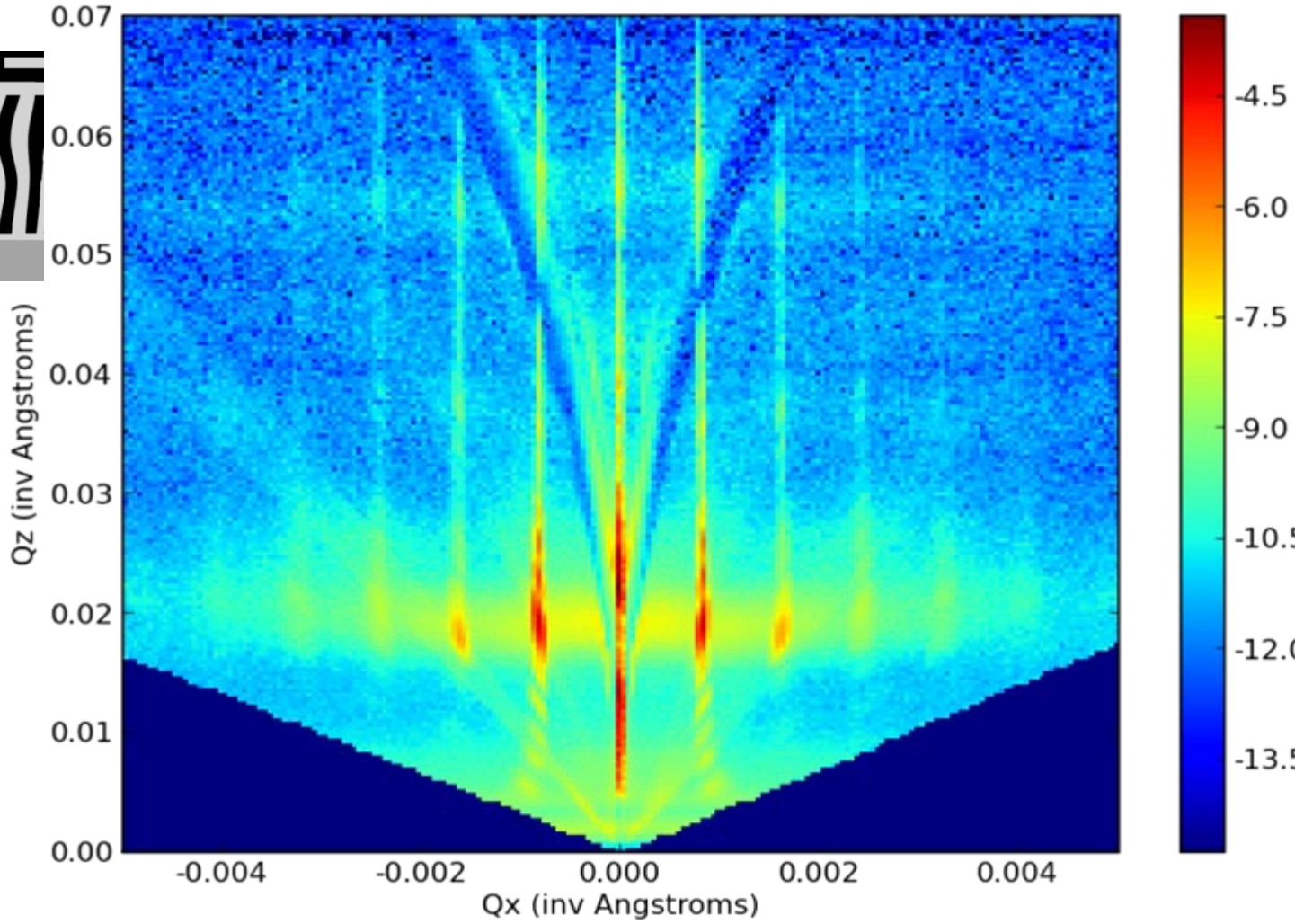


More vertically aligned lamellae



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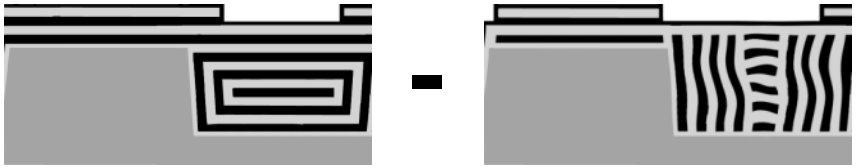

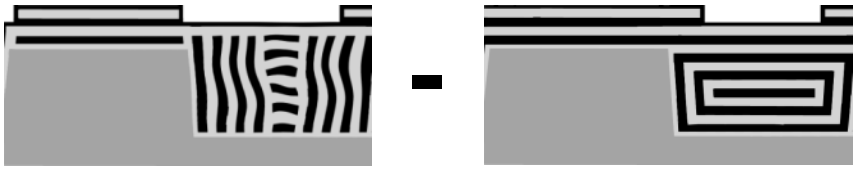

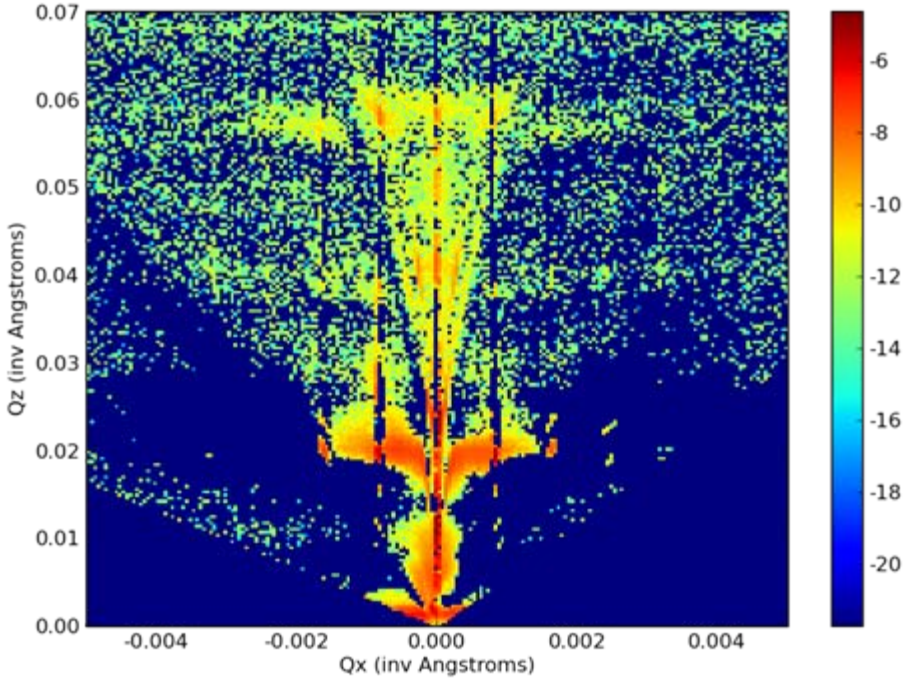

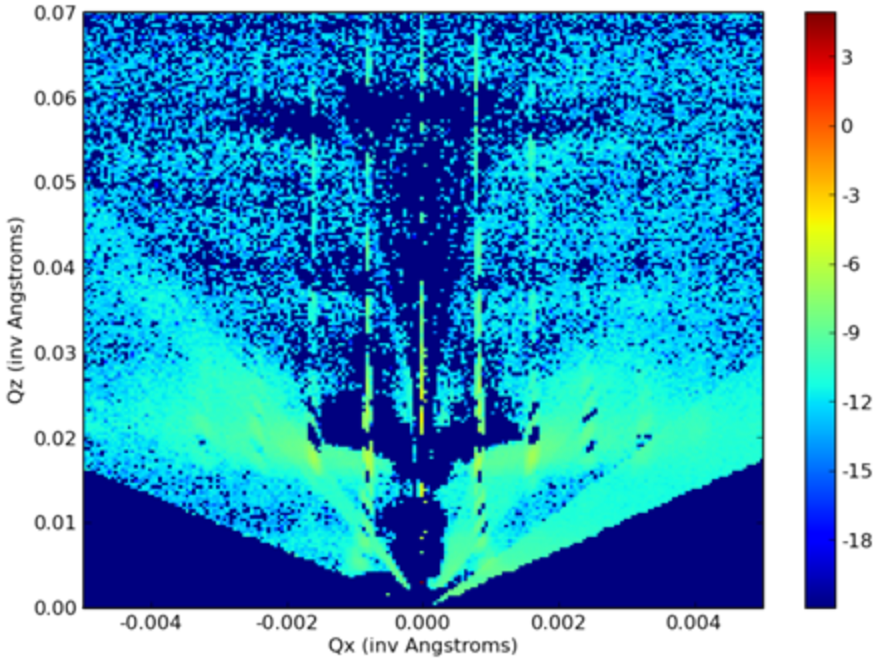

Stronger scattering near Q_x=0, and at high Q_z

Stronger at high Q_x

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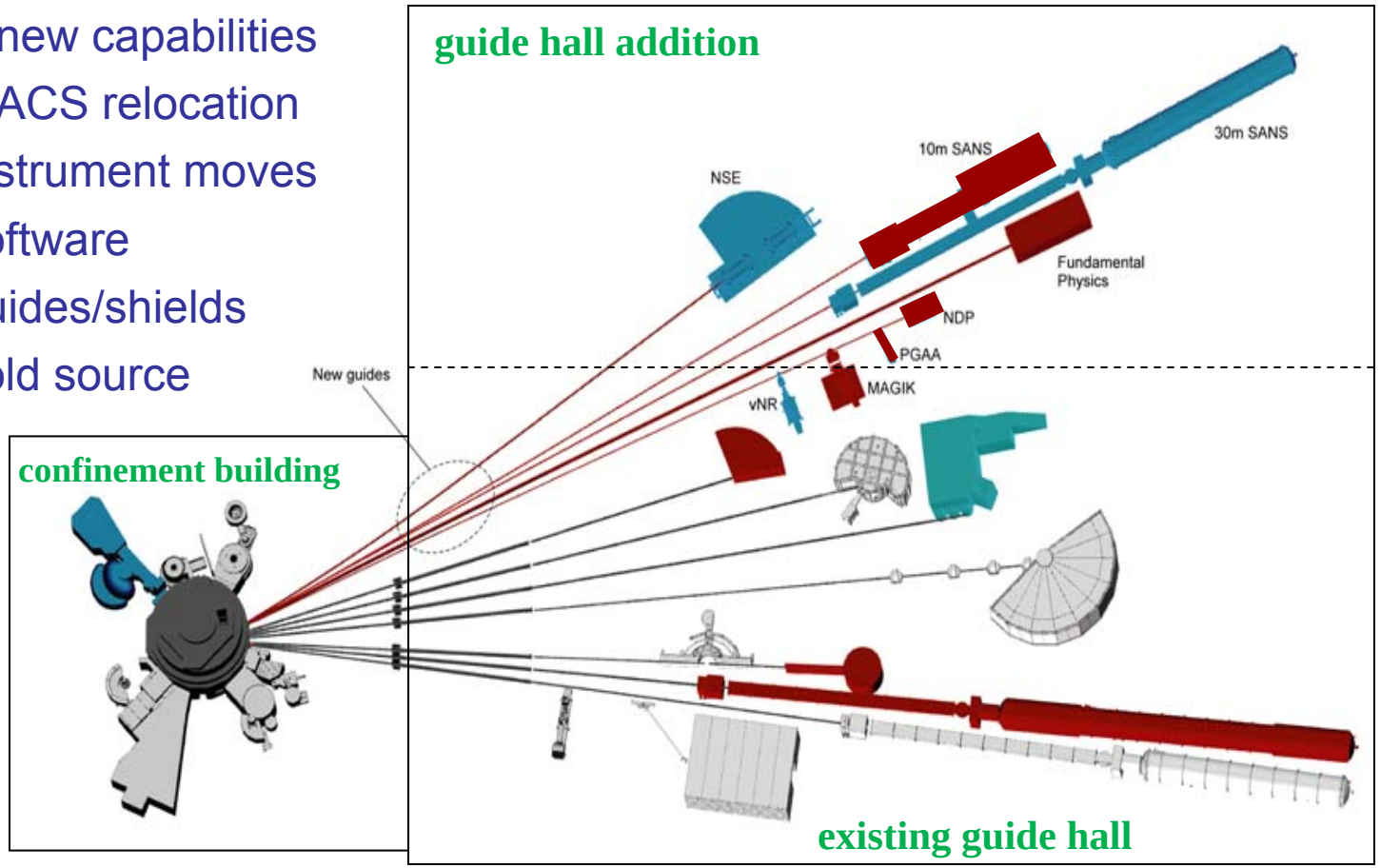
Expansion Activities

- New Cold Source
- Construction
- Instrument development
- Beam delivery
- Reactor reliability enhancements

NCNR Expansion

Many sub-projects:

5 new capabilities
MACS relocation
instrument moves
software
guides/shields
cold source

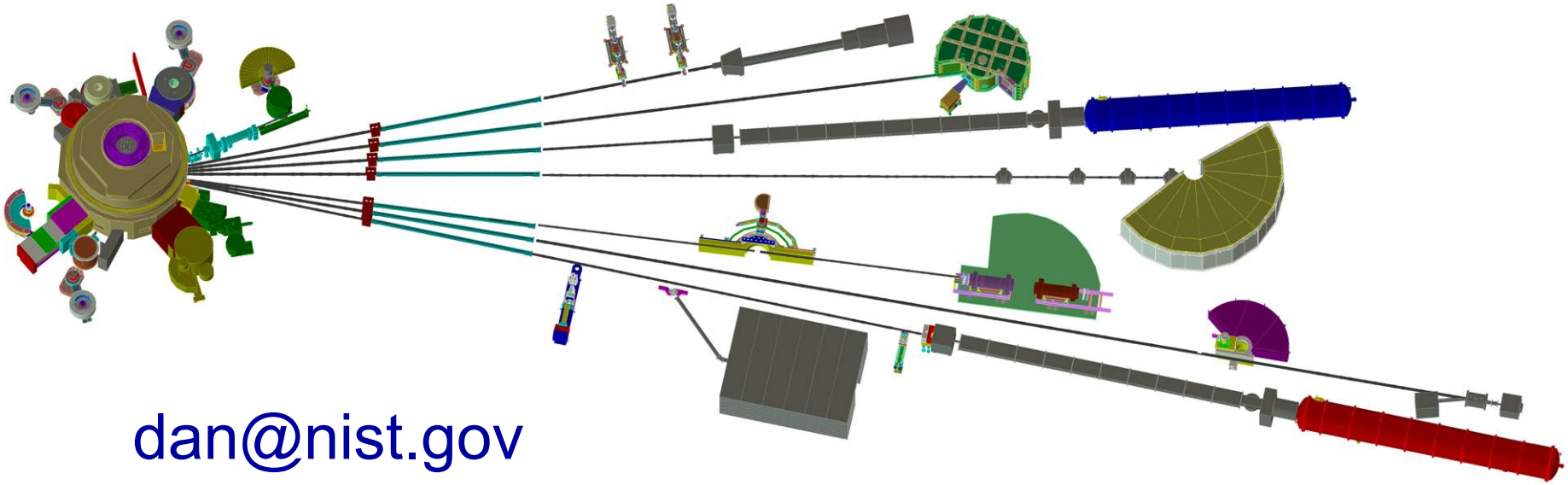


Major areas of activity:

Construction
Cold source
Guide systems
Shield systems
Instruments
Control room upgrade

Neutron methods are extremely versatile

Have a great week!



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Thank you
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