Role of neutrons to determine the bulk properties of complex liquid mixtures

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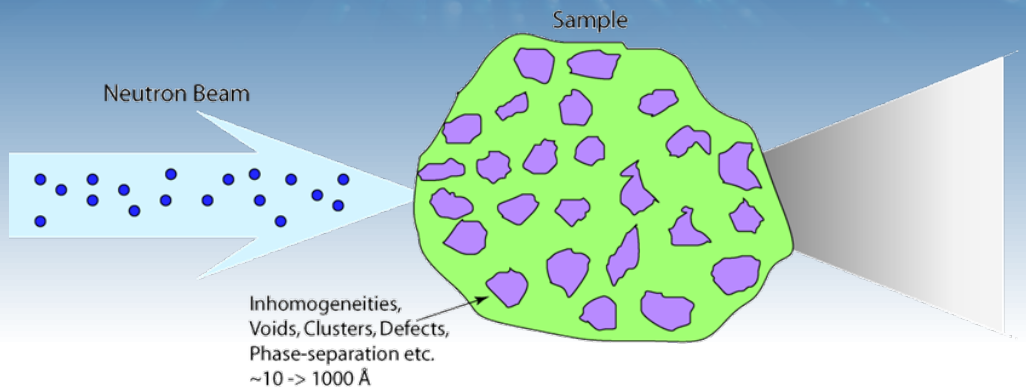
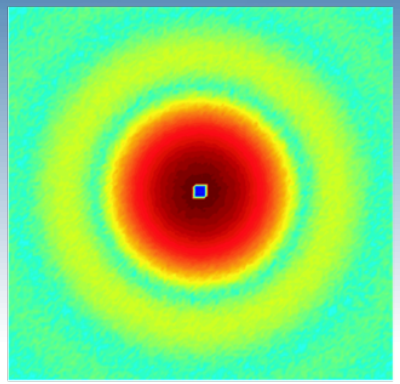
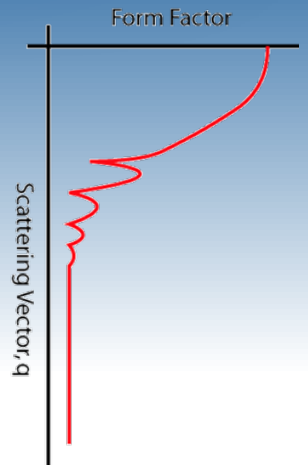
Small Angle Neutron Scattering







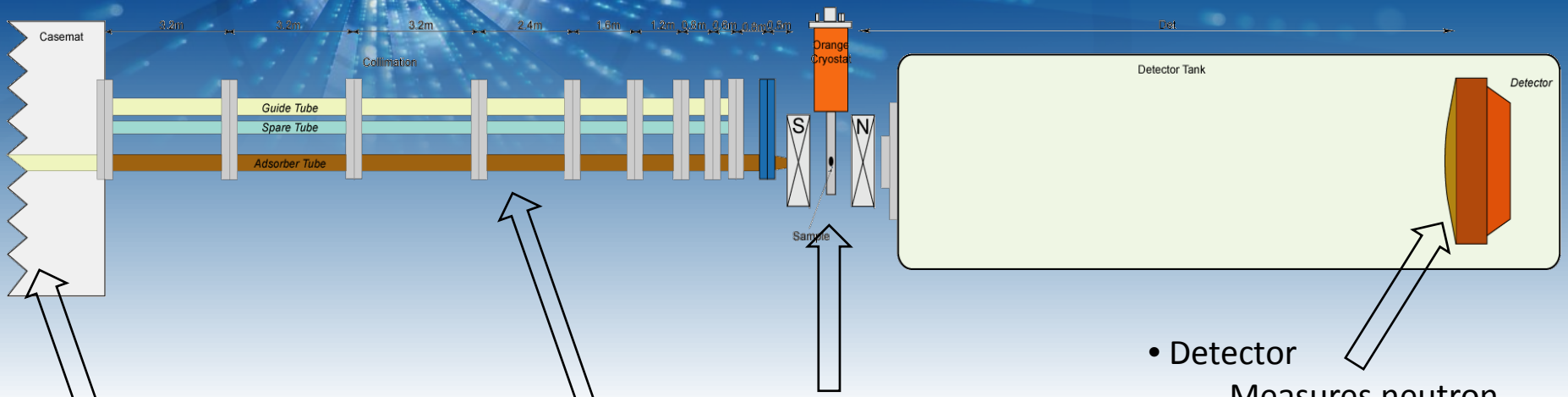
• **Fourier Transform of the particle shape function**

• Scattering methods for '**dilute'** samples return the **'form-factor'** for the ensemble of scattering objects

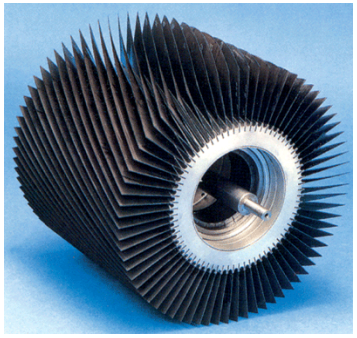
Form-Factor = Fourier transform of the shape function describing the scattering objects

• Scattering from '**concentrated'** samples involves a convolution of the particle form-factor with their interaction '**structure factor'**

Key elements of a SANS instrument….

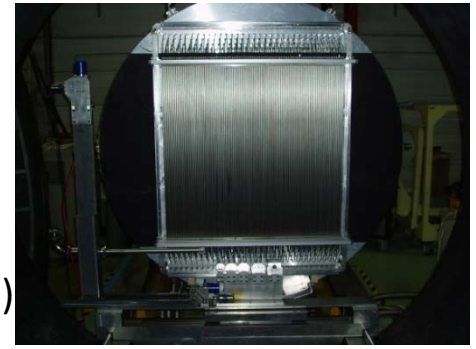


- Velocity selector:
  Extracts a monochromatic neutron beam with broad $\delta\lambda/\lambda$

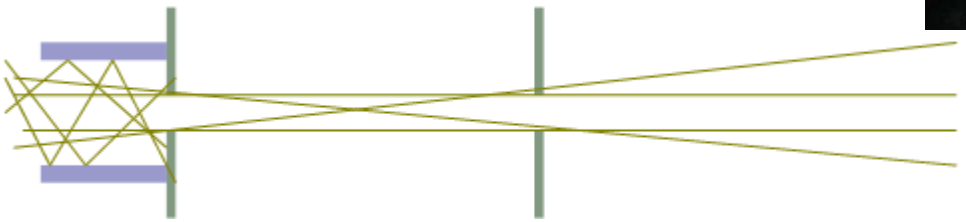


- Sample

- Detector
  Measures neutron scattered from the sample



- Beam collimation:
  Defines a beam divergence (i.e. angular spread of the neutron beam)



D22: simply the best….

- flux (~10^8 n cm^{-2} s^{-1} max)
- dynamic *q*-range ~ 10 - 15
- high count rate detector ~MHz
- polarisation & analysis developments
- *q*-range: 10^{-3} to 0.85 $Å^{-1}$

Small Angle Neutron Scattering (SANS)

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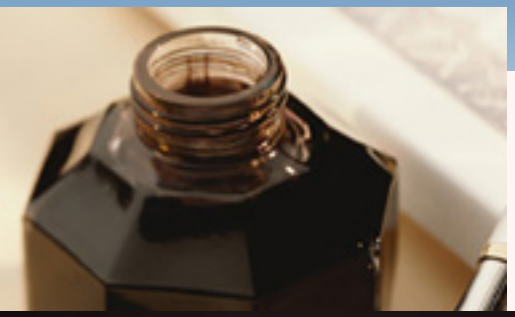
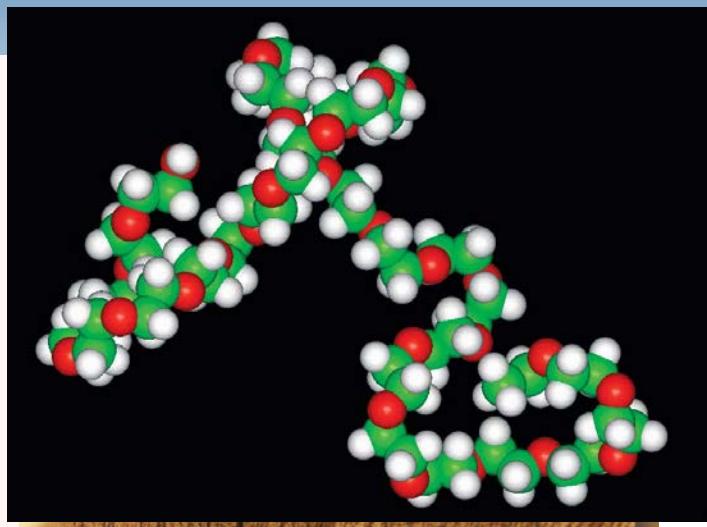
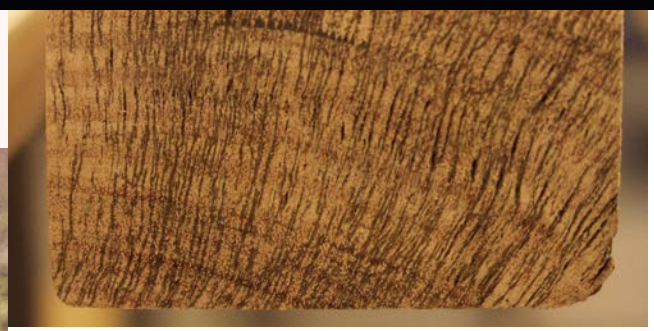
SANS probes Macromolecular and micro structures:
polymers, micelles, complex fluids,
precipitates, porous media, fractal structures

Length scales ~ 1nm - 300nm (20,000nm with USANS)







Contrast Matching with SANS

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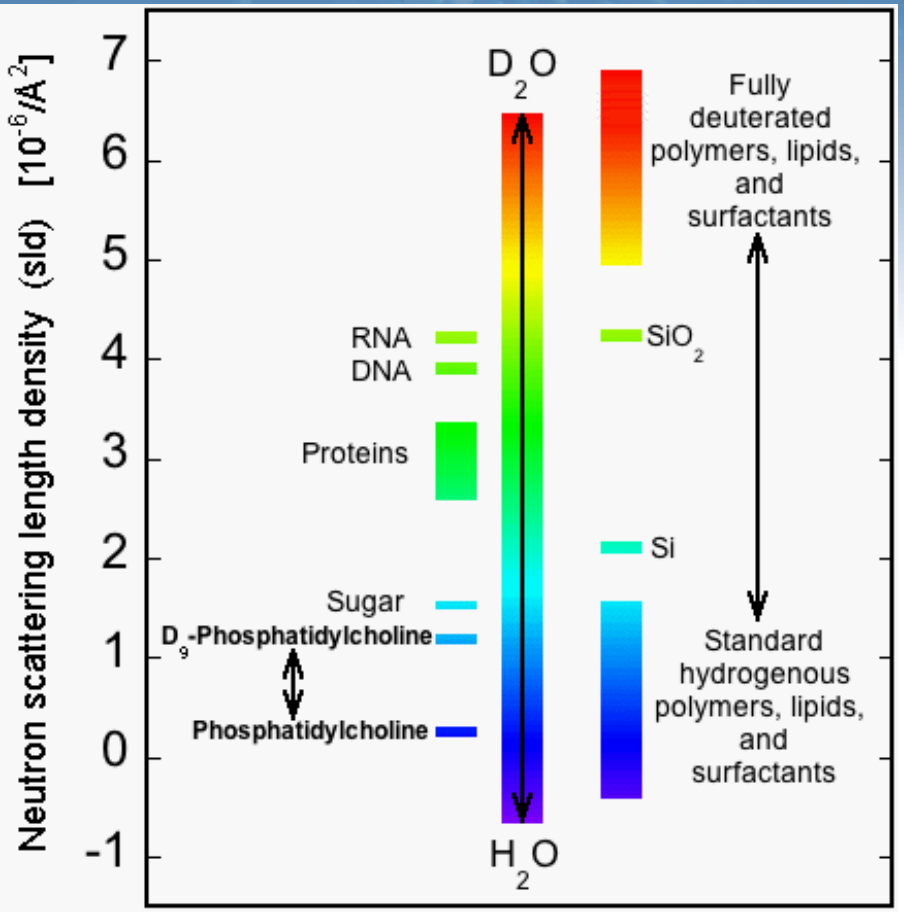
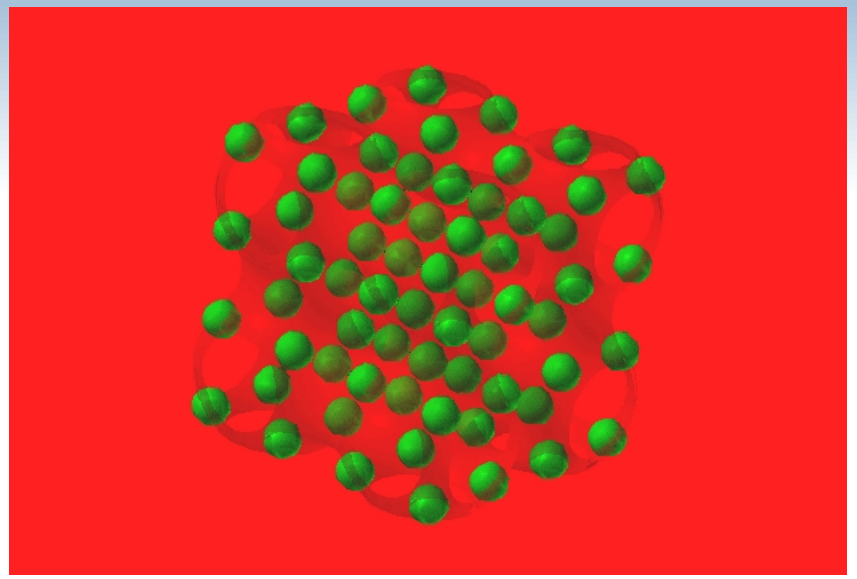
What neutrons see:
Scattering Length Density

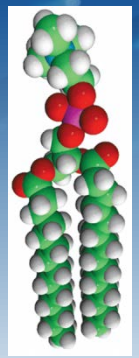


So …
Can H/D contrast match solution & membrane

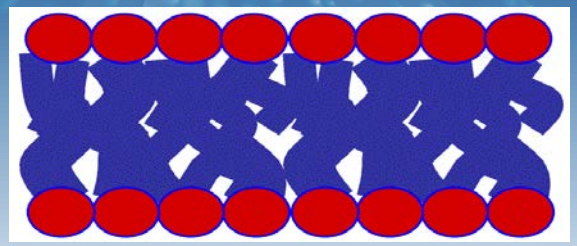


See protein arrangement independents of lipid structure and visa versa

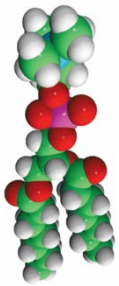
Back to the Bicelles



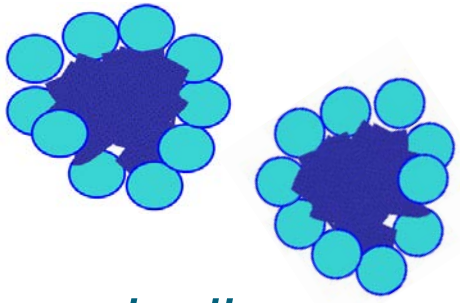
DMPC
14 C chain



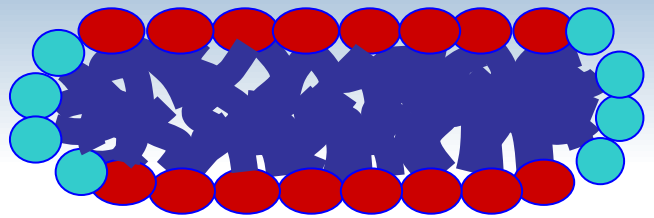
bilayers



DHPC
6 C chain



micelles

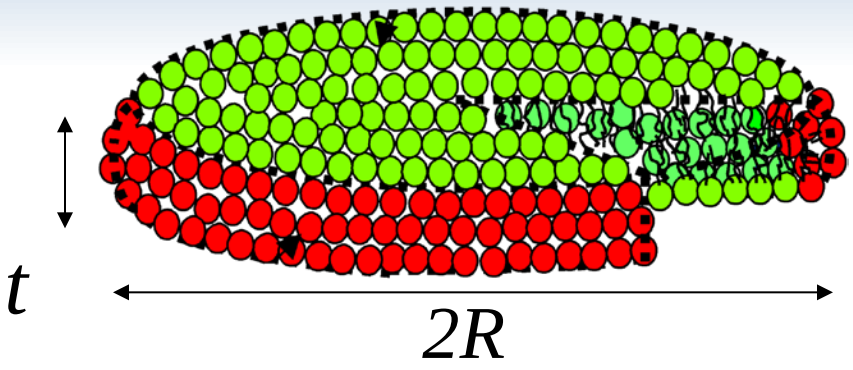


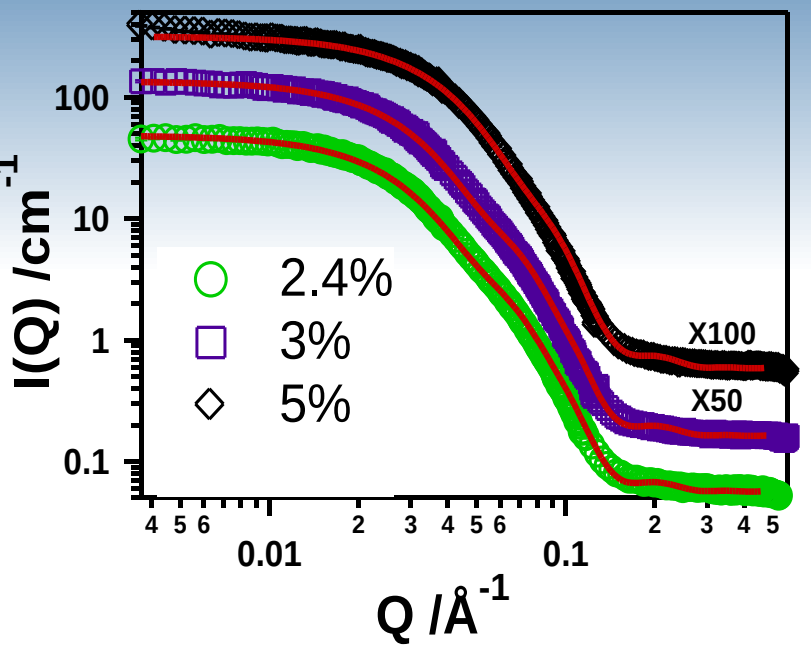
Bilayer + Micelle ⟶ Bicelle

Objective: simple engineering = use cell membrane components to create compatible carriers and canisters

May be they aren't disks…

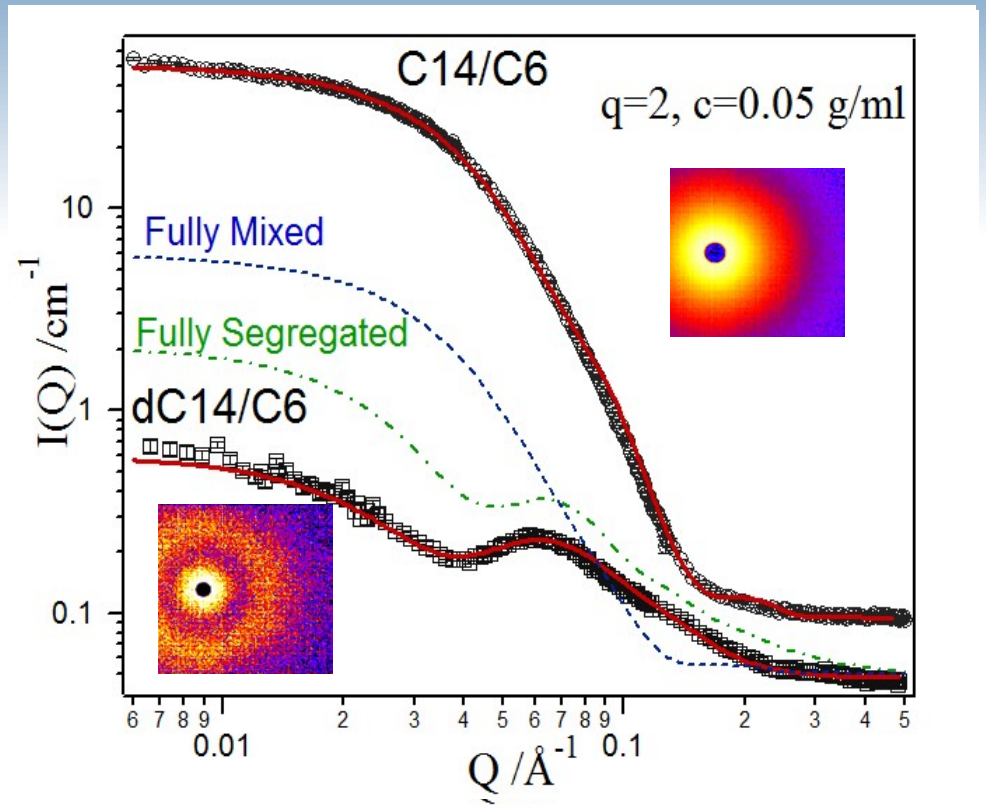
Disc Form factor fit

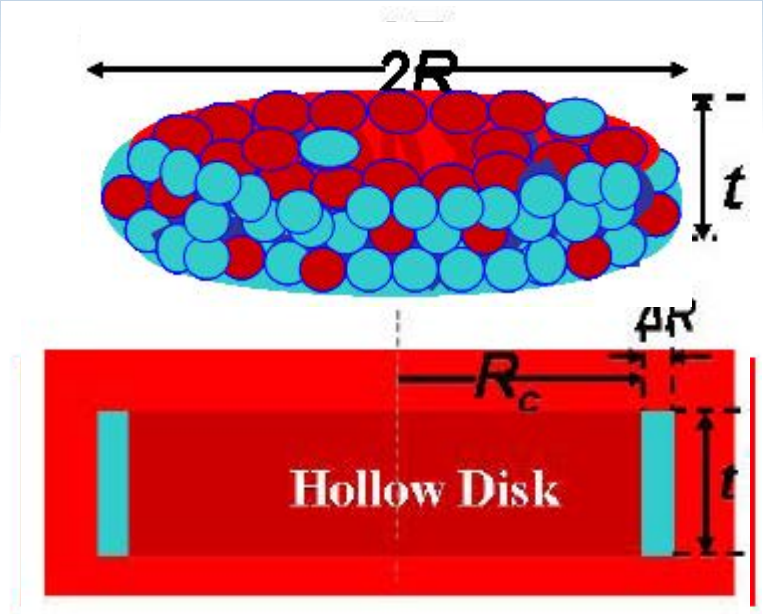




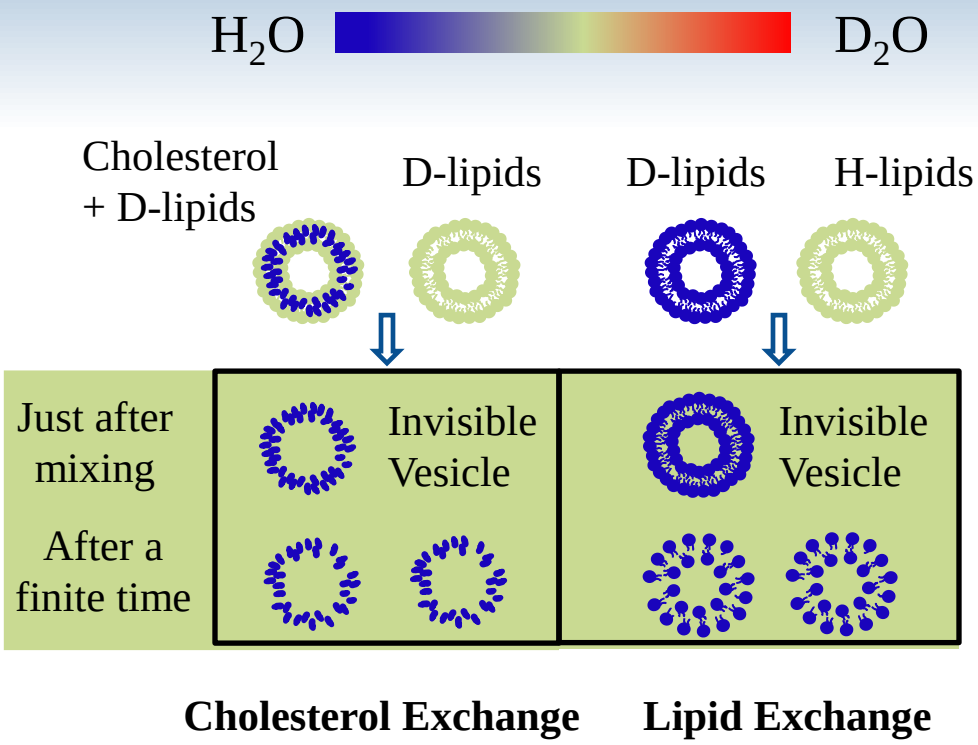
SANS I vs Q is completely consistent with a simple disk as drawn in this cartoon

Mixing/Segregation confirmation





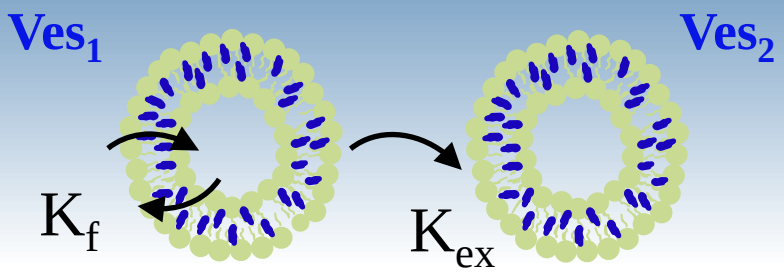
In-situ transfer by Time-Resolved SANS



Advantages:

1) Do not require vesicles isolation (in situ technique)
2) No need of fluorescent or tag cholesterol
3) Access early stage of transfer
4) Accurate control on lipid membrane composition and structure
5) Can be applied to anything (just require deuterated materials)

Time-Resolved SANS approach



Kinetic

$$\frac{dC_{in1}}{dt} = -K_f C_{in1} + K_f C_{out1}$$

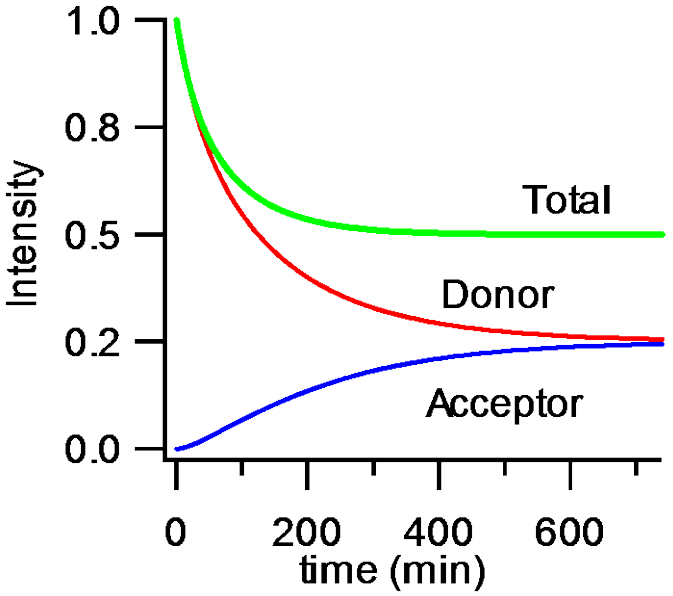
$$\frac{dC_{out1}}{dt} = K_f C_{in1} - K_f C_{out1} - K_{ex} C_{out1} + K_{ex} C_{out2}$$

Scattering

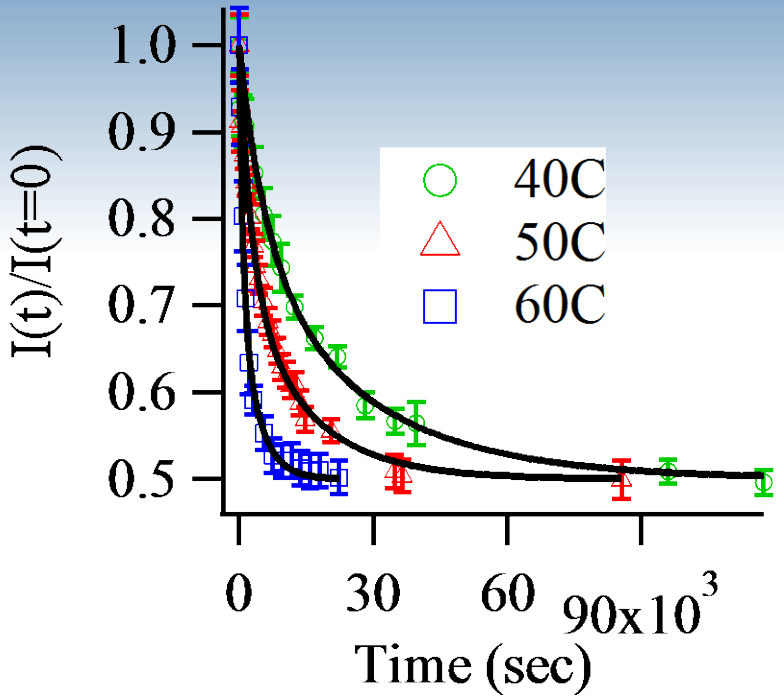
$$I \sim \phi_{Ves1} V_1 \left(SLD_{ves1} - SLD_{solvent}\right)^2 FF$$

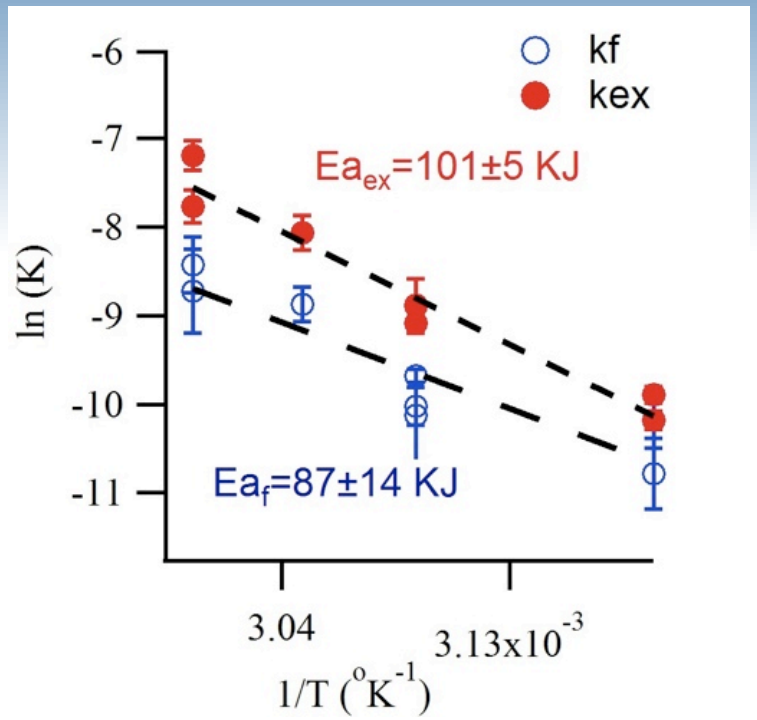
$$+\phi_{Ves2} V_2 \left(SLD_{ves2} - SLD_{solvent}\right)^2 FF$$

$$I \sim \frac{\phi_{Ves}}{2}\left\{\left(\left(\phi_{chol1}^{vol}\right)^2 + \left(\phi_{chol2}^{vol}\right)^2\right)\left[SLD_{Chol} - SLD_{solvent}\right]^2\right\}$$



Cholesterol's transfer in POPC vesicles

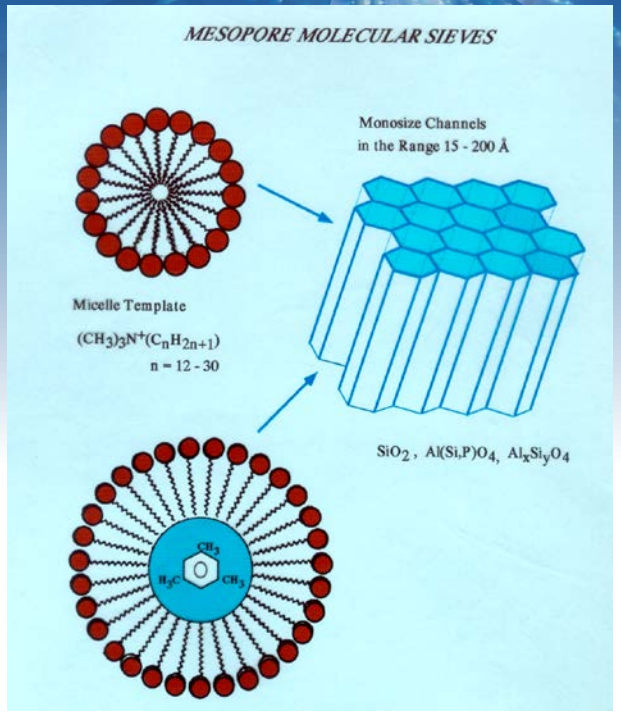


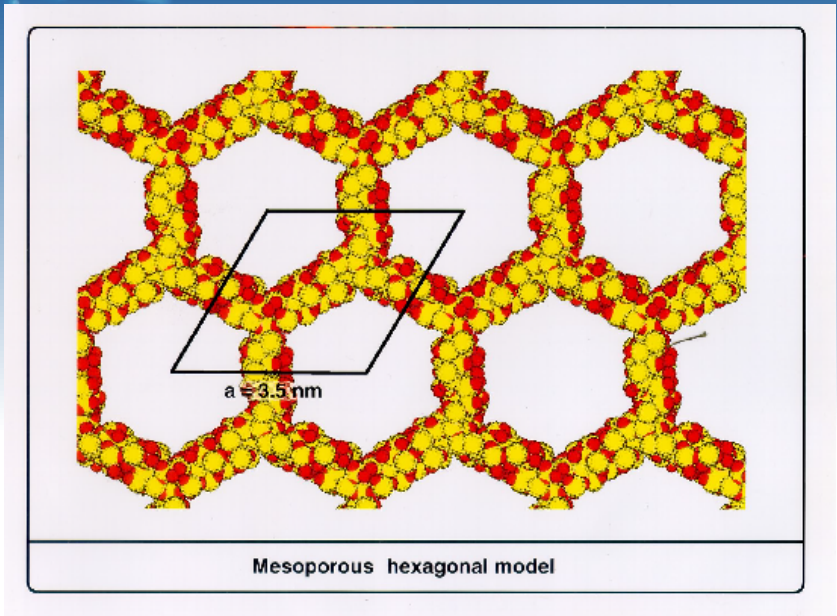


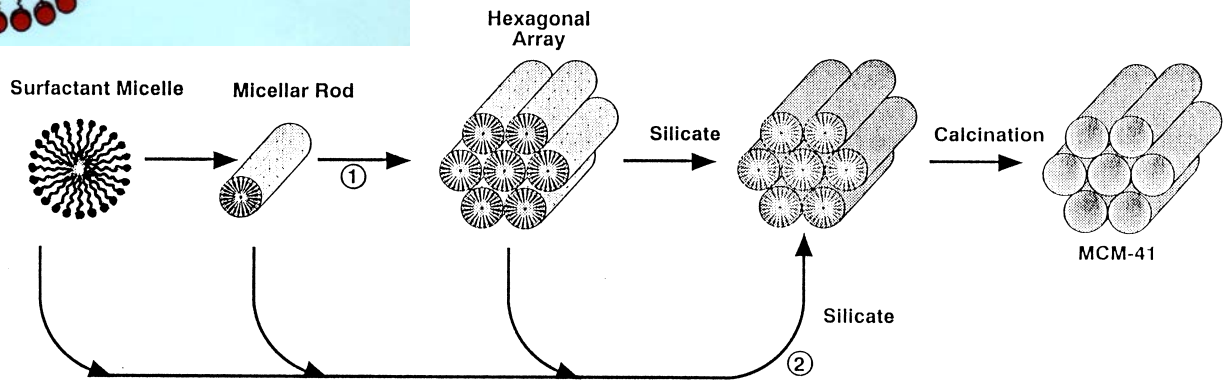
Half life for exchange: ~100min
Half life for flipping: ~250min (surprisingly slow)

Total cholesterol exchange!!

Structure and Formation of MCM-41 Mesoporous Silica

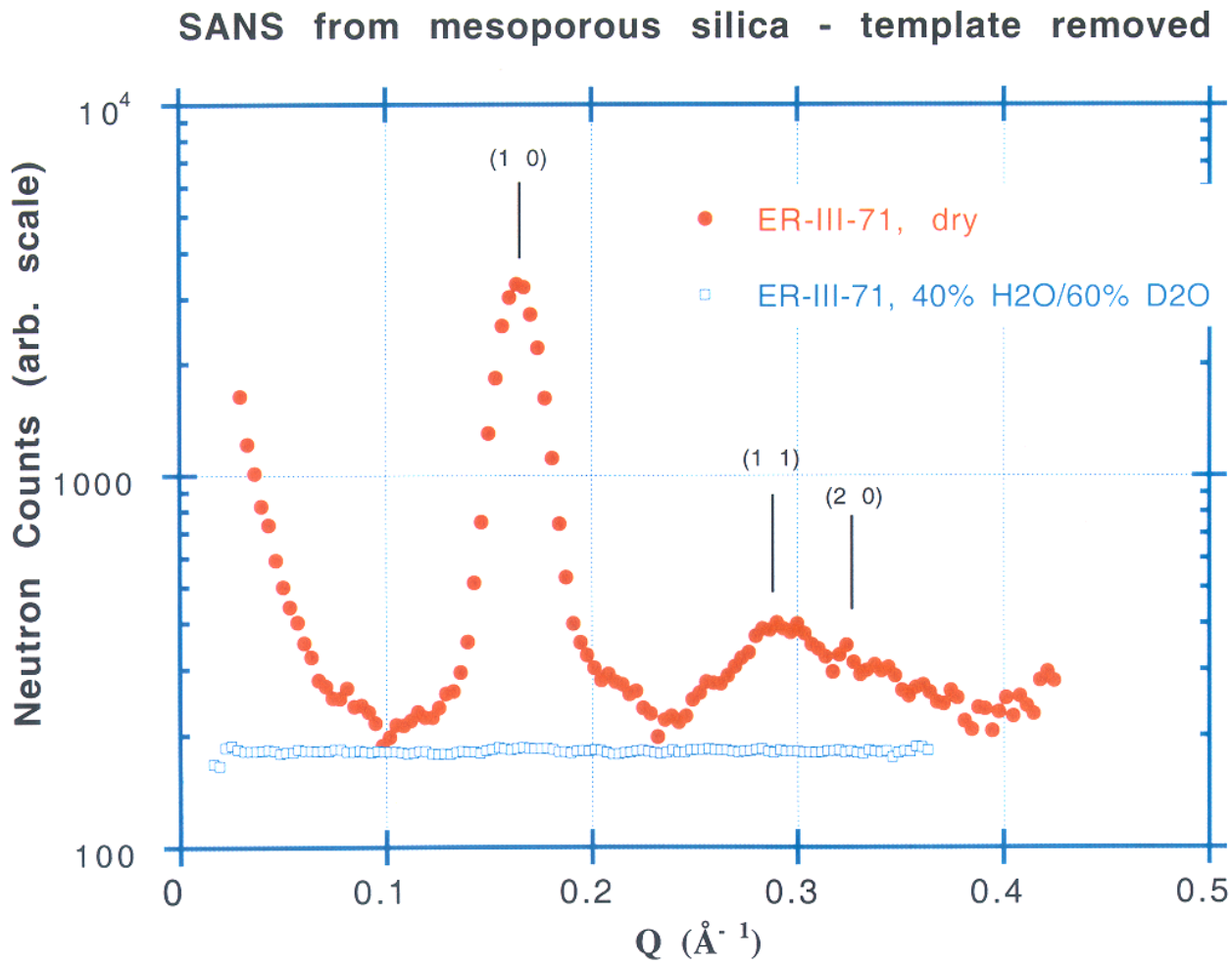






First Proposed mechanism – Kresge, et al. *NATURE* **359**, 710 (1992).

Structure and Formation of MCM-41 Mesoporous Silica



Pores completely filled by null contrast fluid

* C. Glinka, et al. *J.Porous Matls.* **3**, 93 (1996)