

Diffuse X-ray Scattering Provides
More and Better Information About
Biomembranes than Traditional
Diffraction Methods

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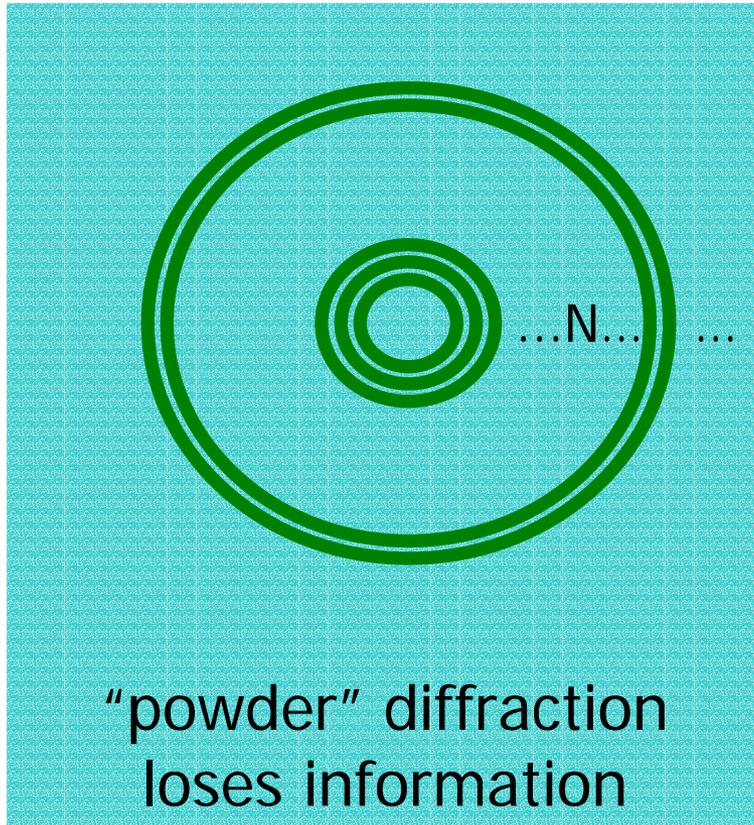
<http://lipid.phys.cmu.edu> for papers

Samples

“Old” method – BBA 2000

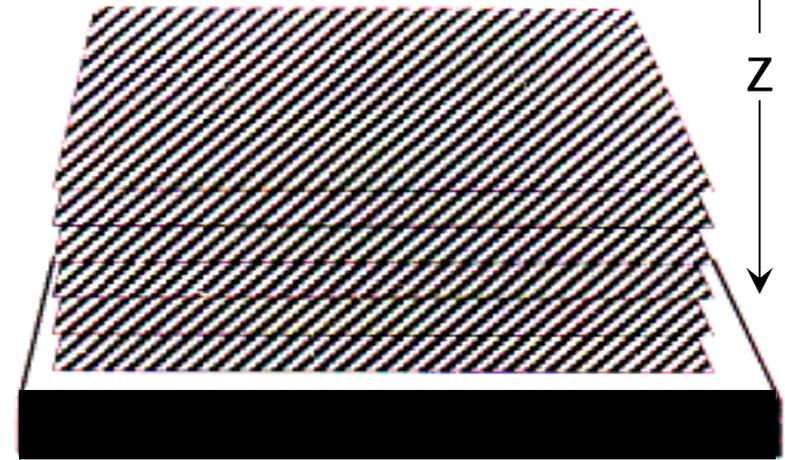
MLVs

Multilamellar vesicles



Oriented

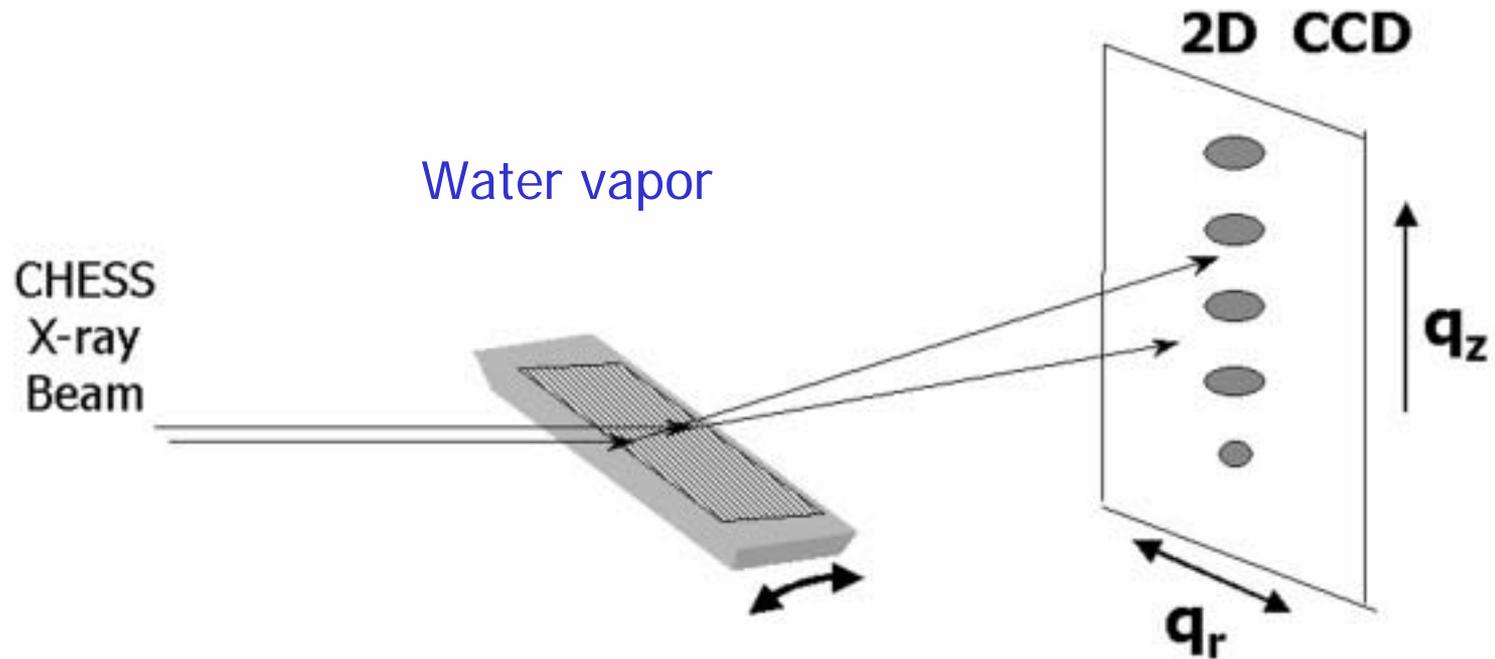
Stacks of 800-2000 Lipid Bilayers



More intensity and spatial information

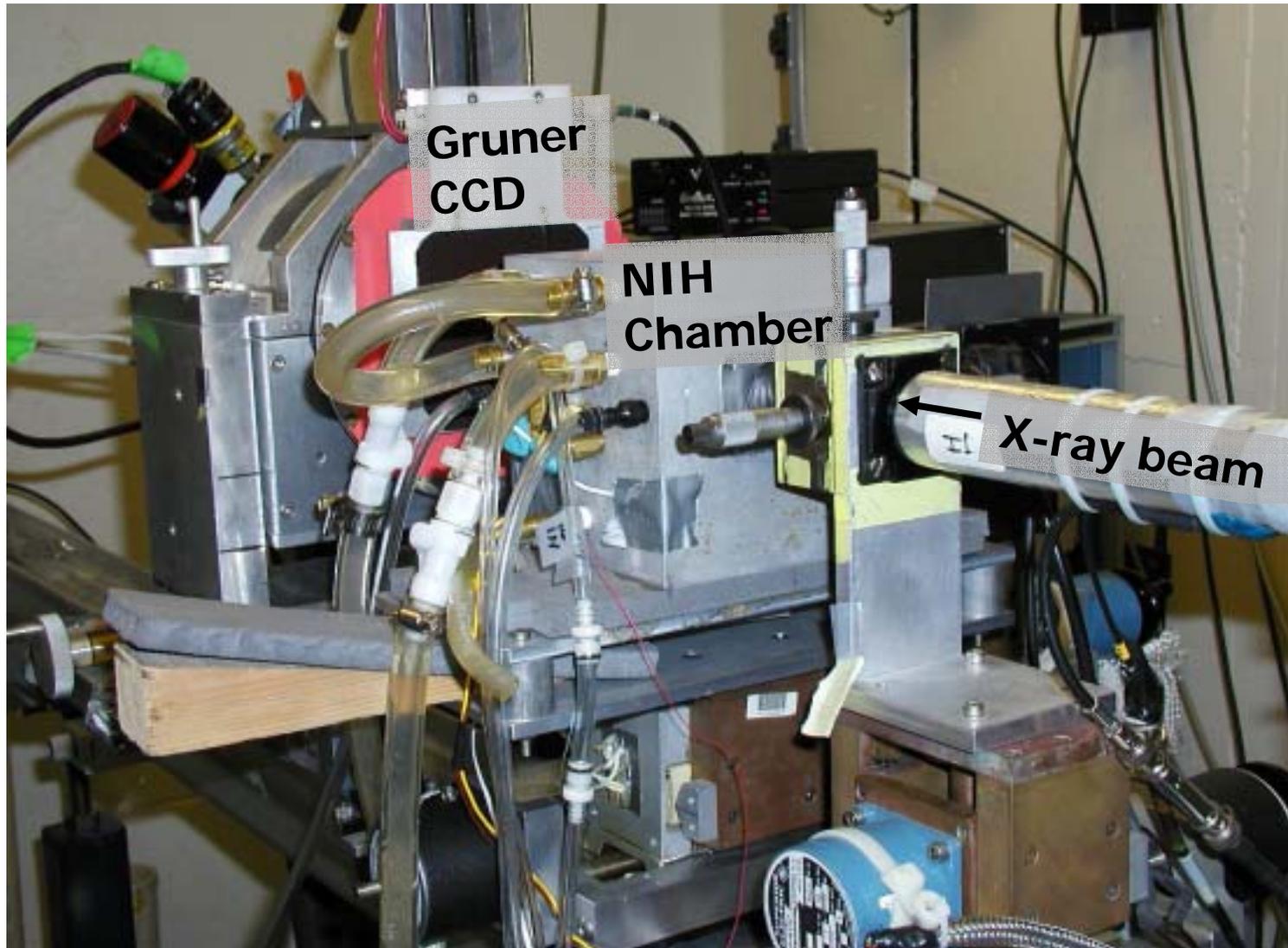
Full hydration is achieved from the vapor.

Experimental Geometry

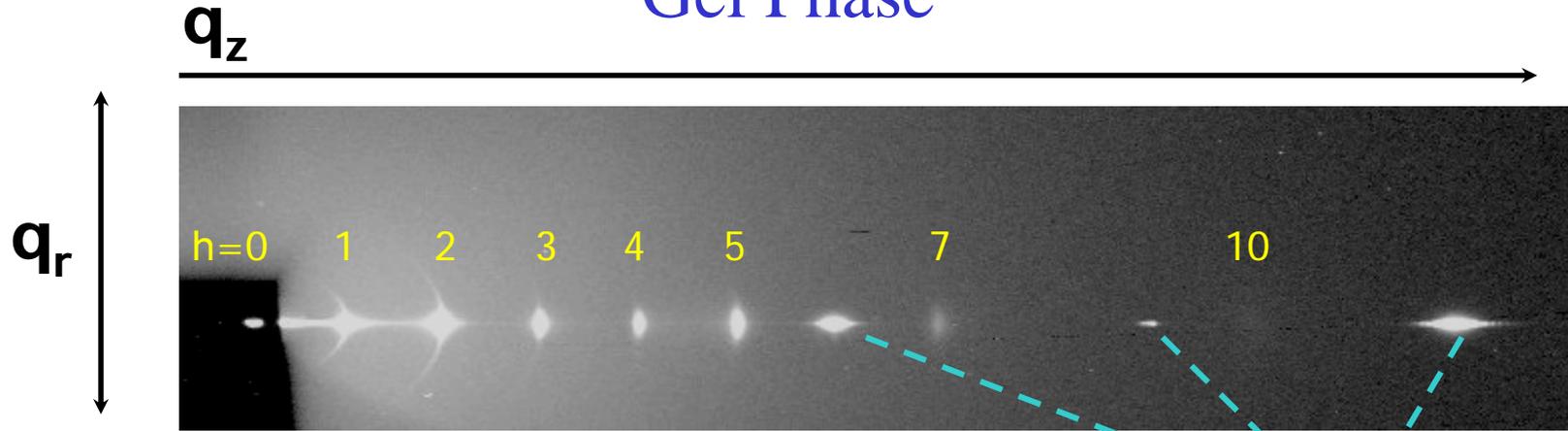


Oriented sample prepared by
ROCK and ROLL method
on a flat substrate which is rotated
during data collection

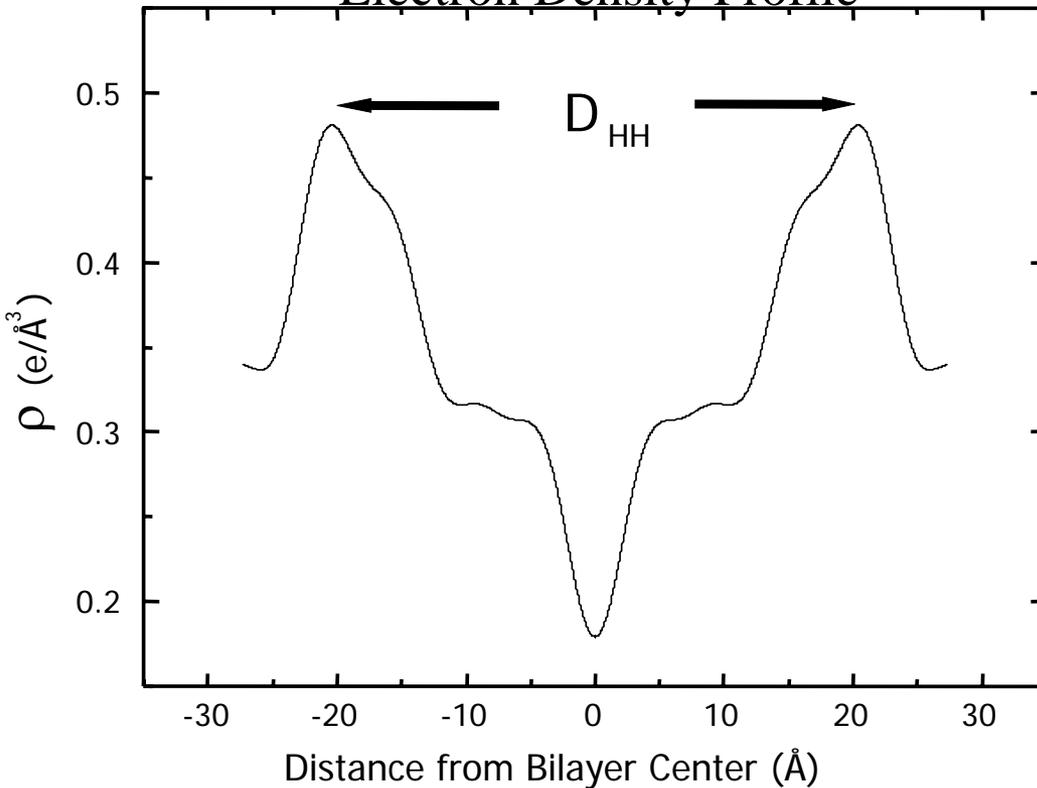
D1 Hutch at CHESS



Gel Phase



Electron Density Profile



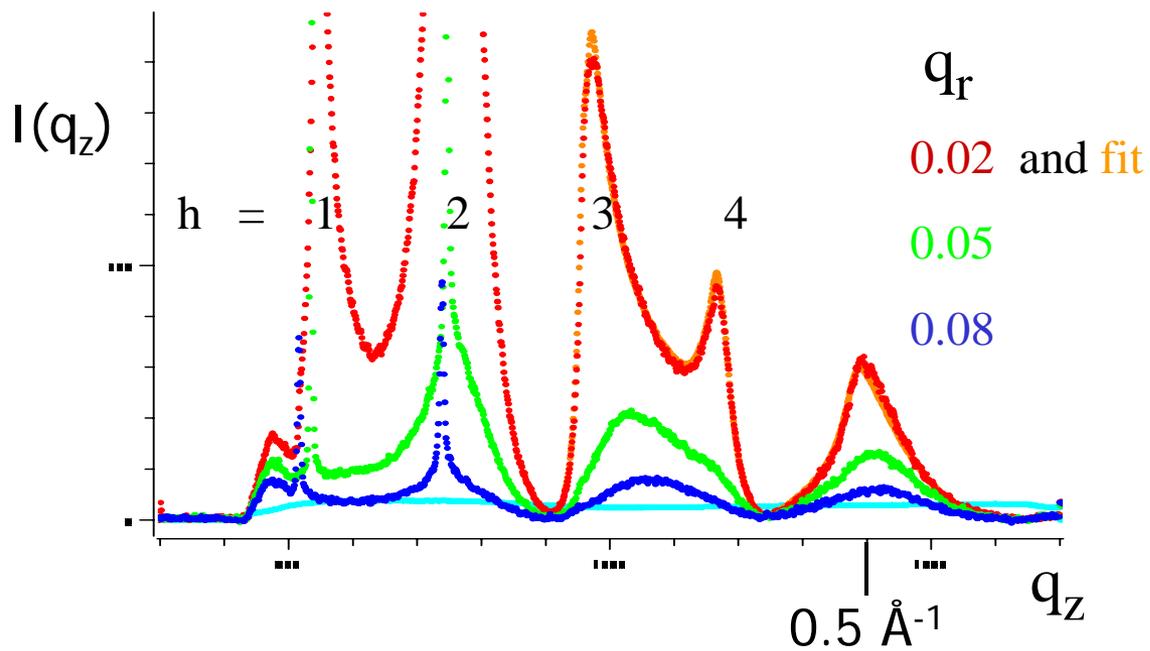
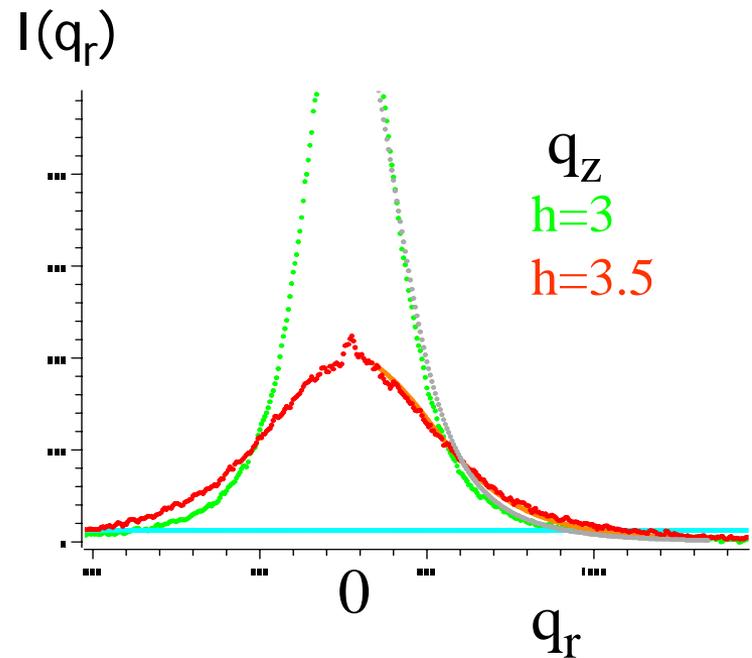
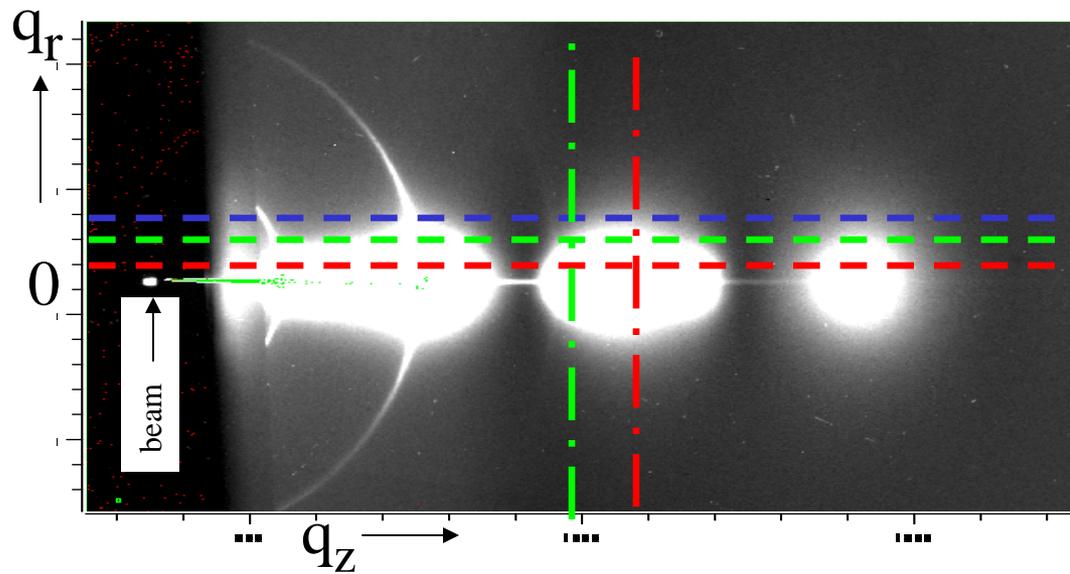
Mica peaks
from substrate

$$I_h = |F(\frac{2\pi h}{D})|^2 / (\frac{2\pi h}{D})$$

$$\rho(z) = \sum_h F(\frac{2\pi h}{D}) \cos(\frac{2\pi h z}{D})$$

Biophys J (2002) 83: 3324
for enhanced analysis

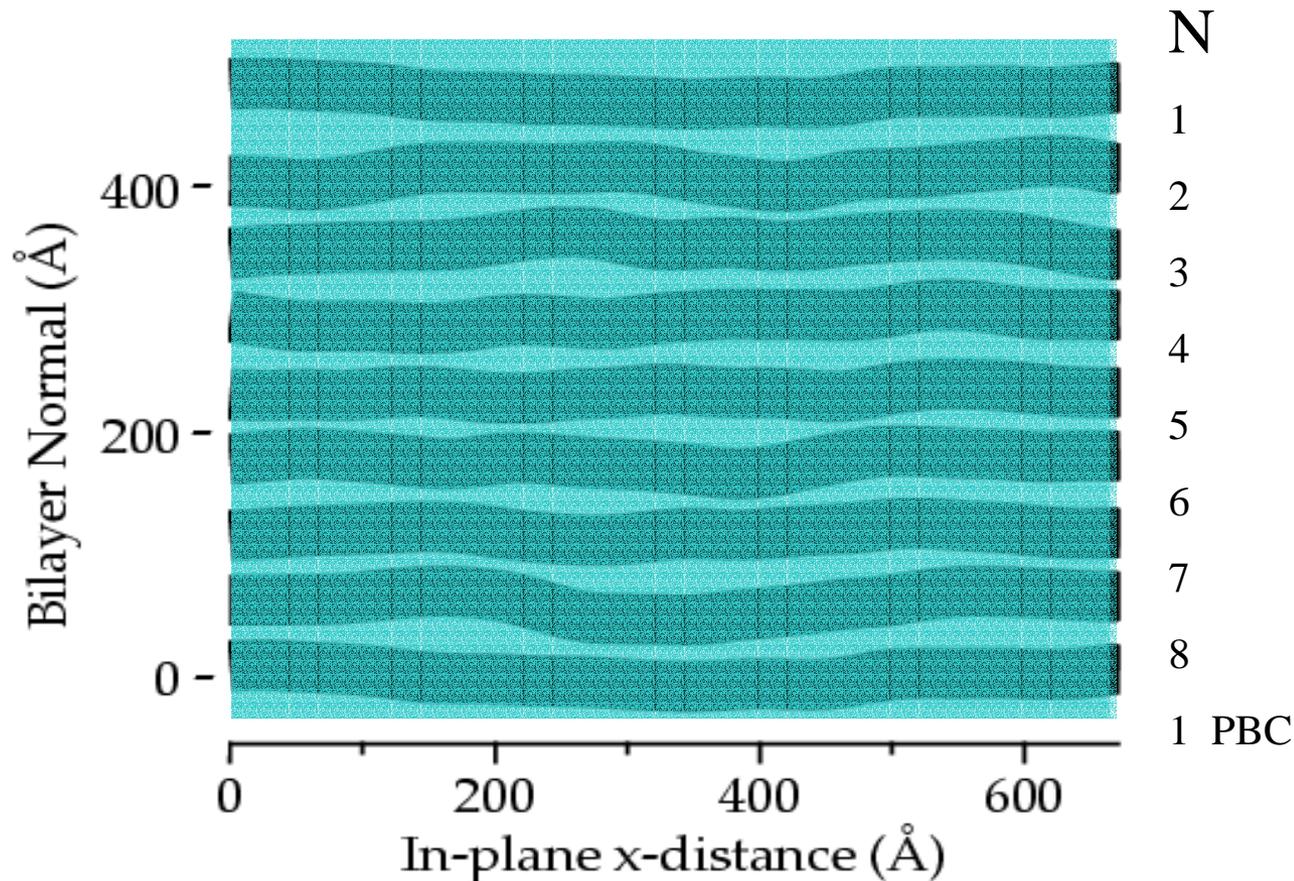
Fluid L_α Phase



Fluctuations cause diffuse scattering: more information than in the peaks!

Cause of diffuse scattering– disorder of second kind

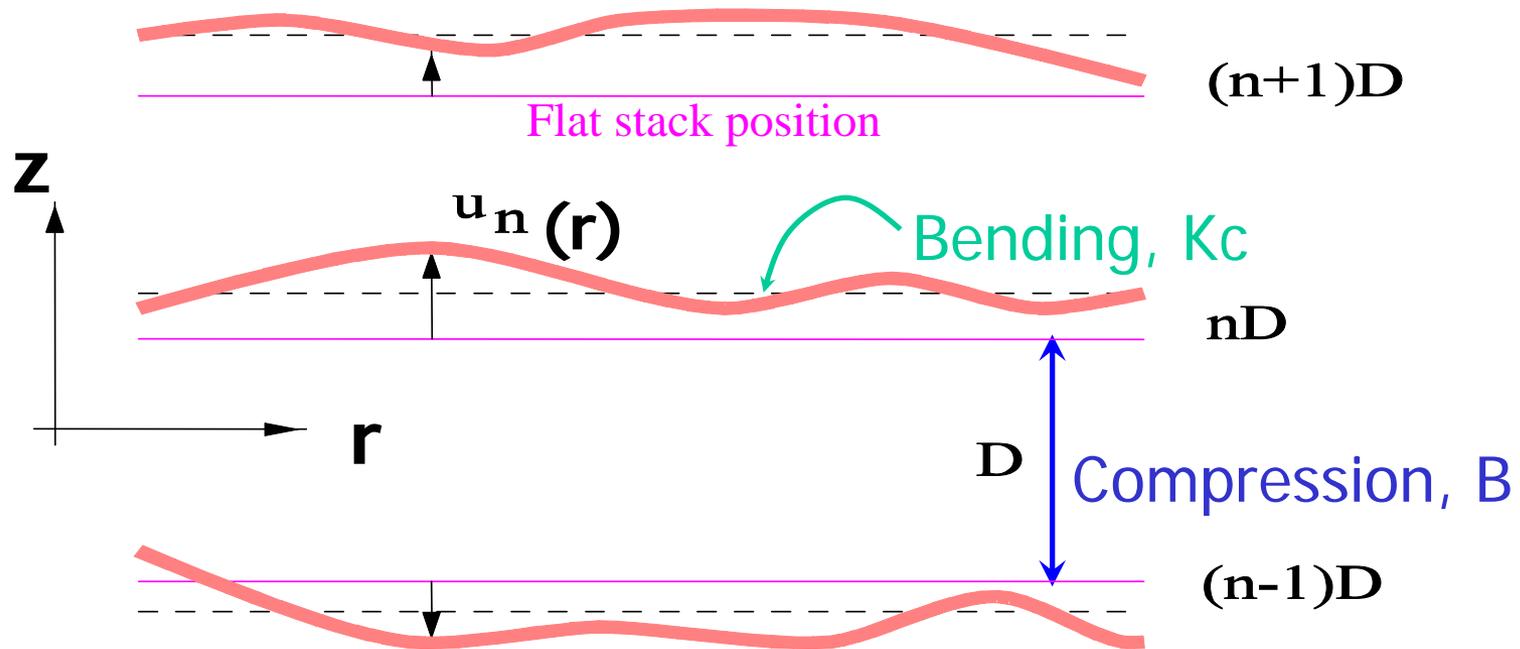
Fluctuations - Interbilayer



Our Monte Carlo **Mesoscale** Simulation with bending and van der Waals and hydration **Interactions**

Theory – Smectic Liquid Crystals

DeGennes

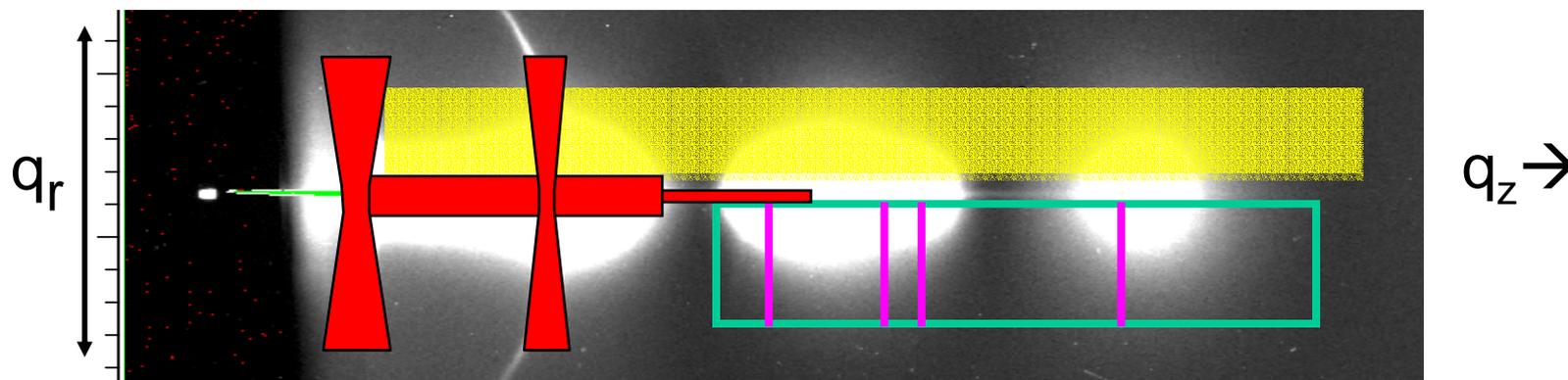
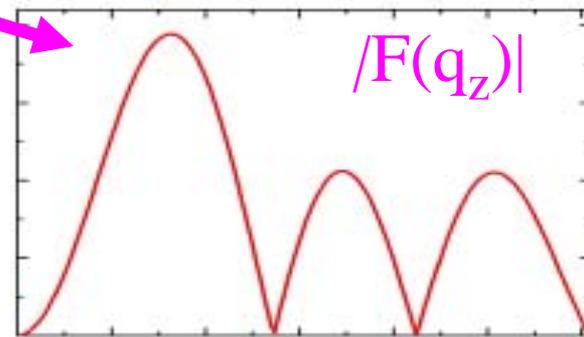
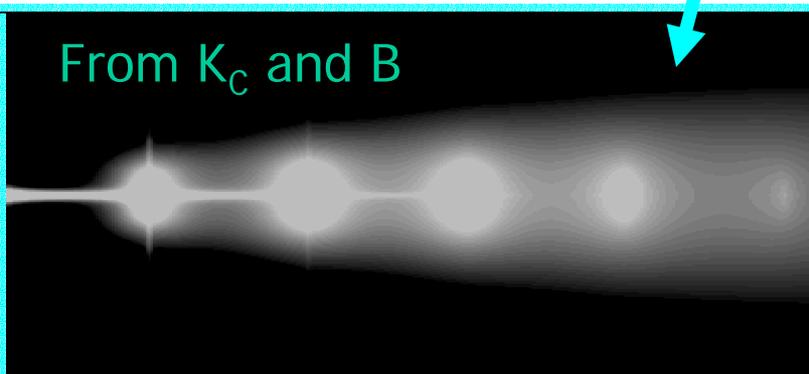


$$f_{fluc} = \frac{\pi}{NL^2} \int r dr \sum_{n=0}^{N-1} [K_c (\nabla_r^2 u_n(r))^2 + B (u_{n+1}(r) - u_n(r))^2]$$

Caille worked out $S(q)$ implications

Data Analysis in the New Method -

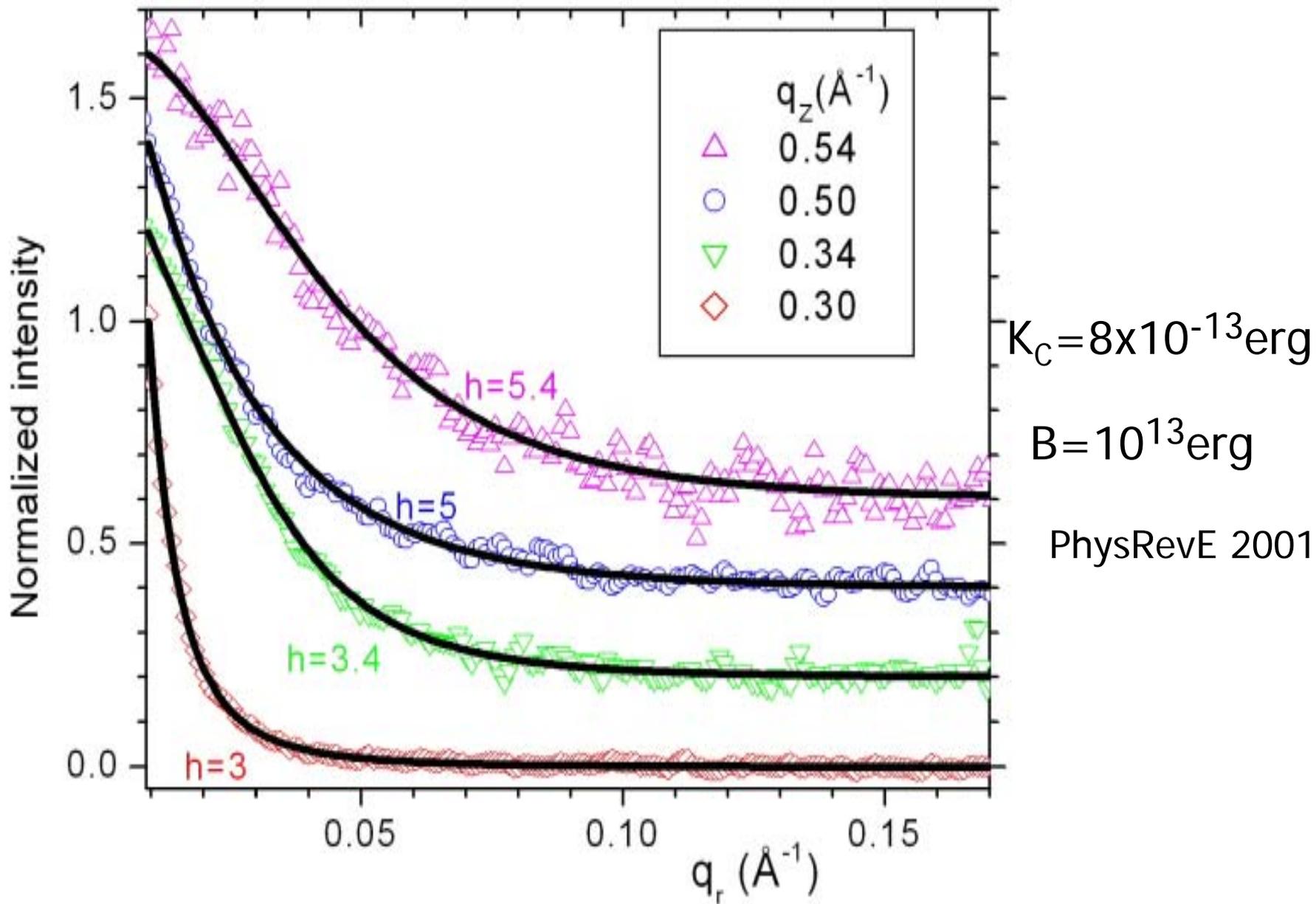
Reminder: $I(\mathbf{q}) = S(\mathbf{q}) |F(q_z)|^2/q_z \rightarrow I(q_r) = S(q_r) \text{ const}$



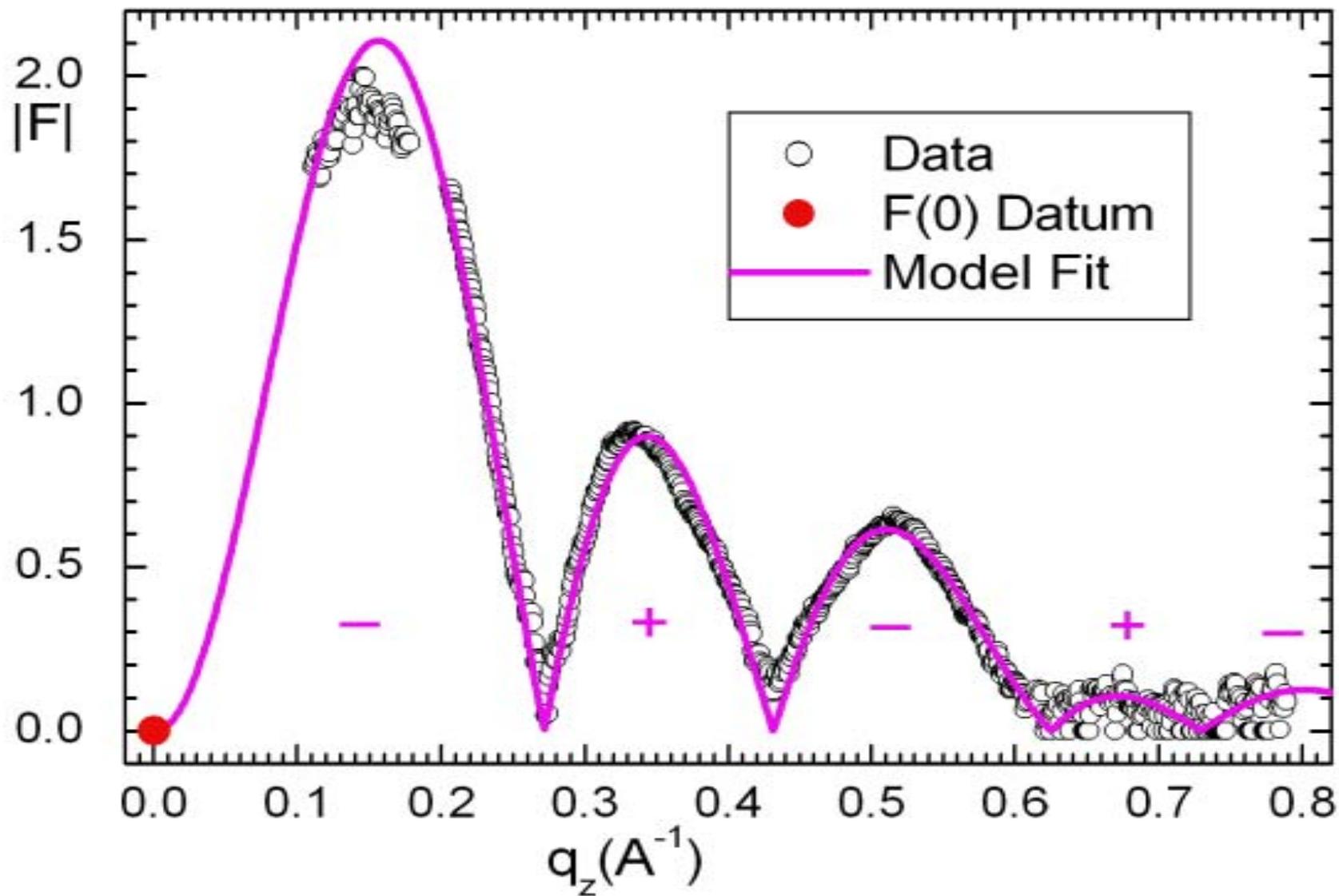
Fitting along q_r determines K_C , B and $S(\mathbf{q}) \rightarrow$ INTERACTIONS

constants give $F(q_z) \rightarrow$ STRUCTURE

$I(q_r)$ Fits



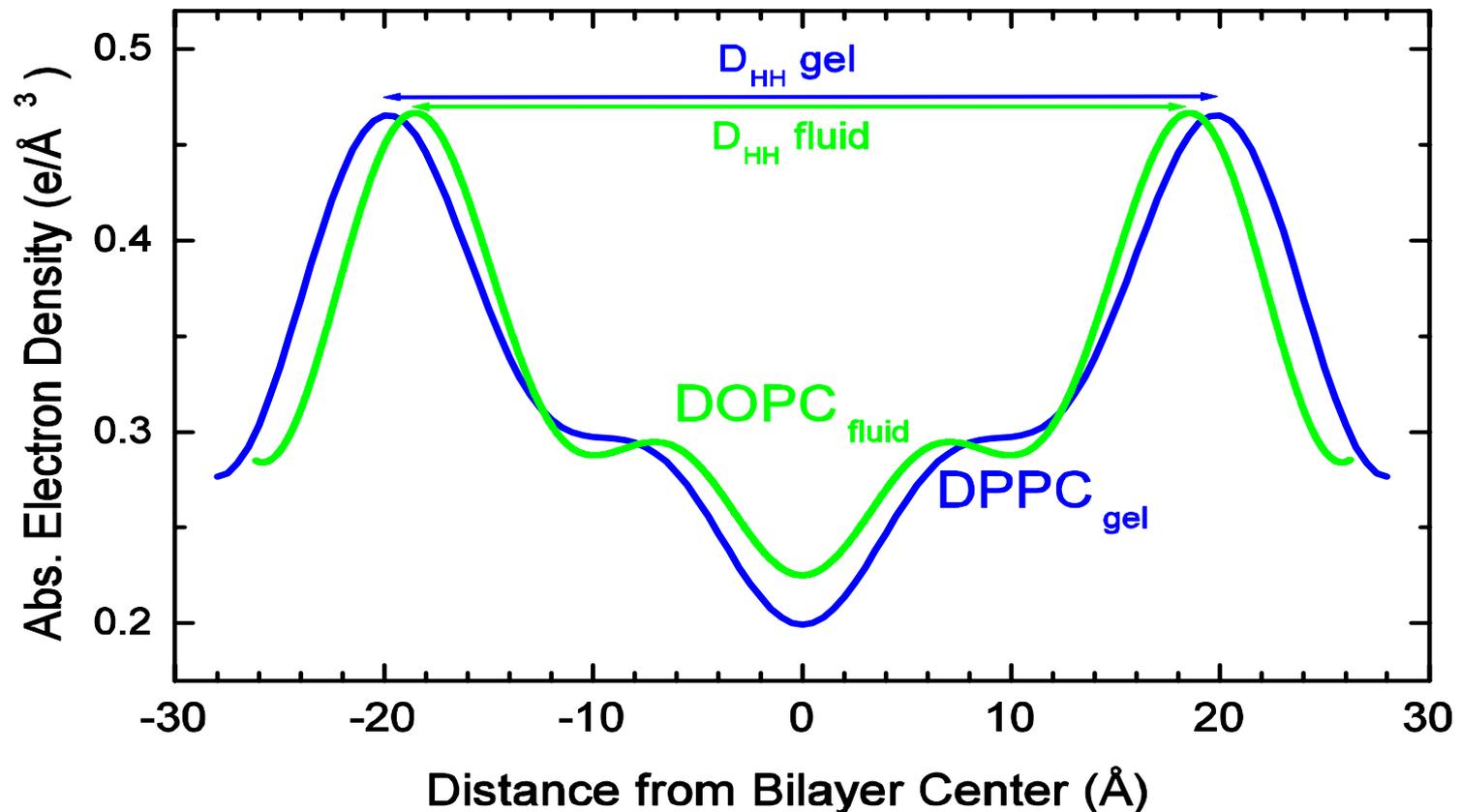
$F(q_z)$ and fit to model



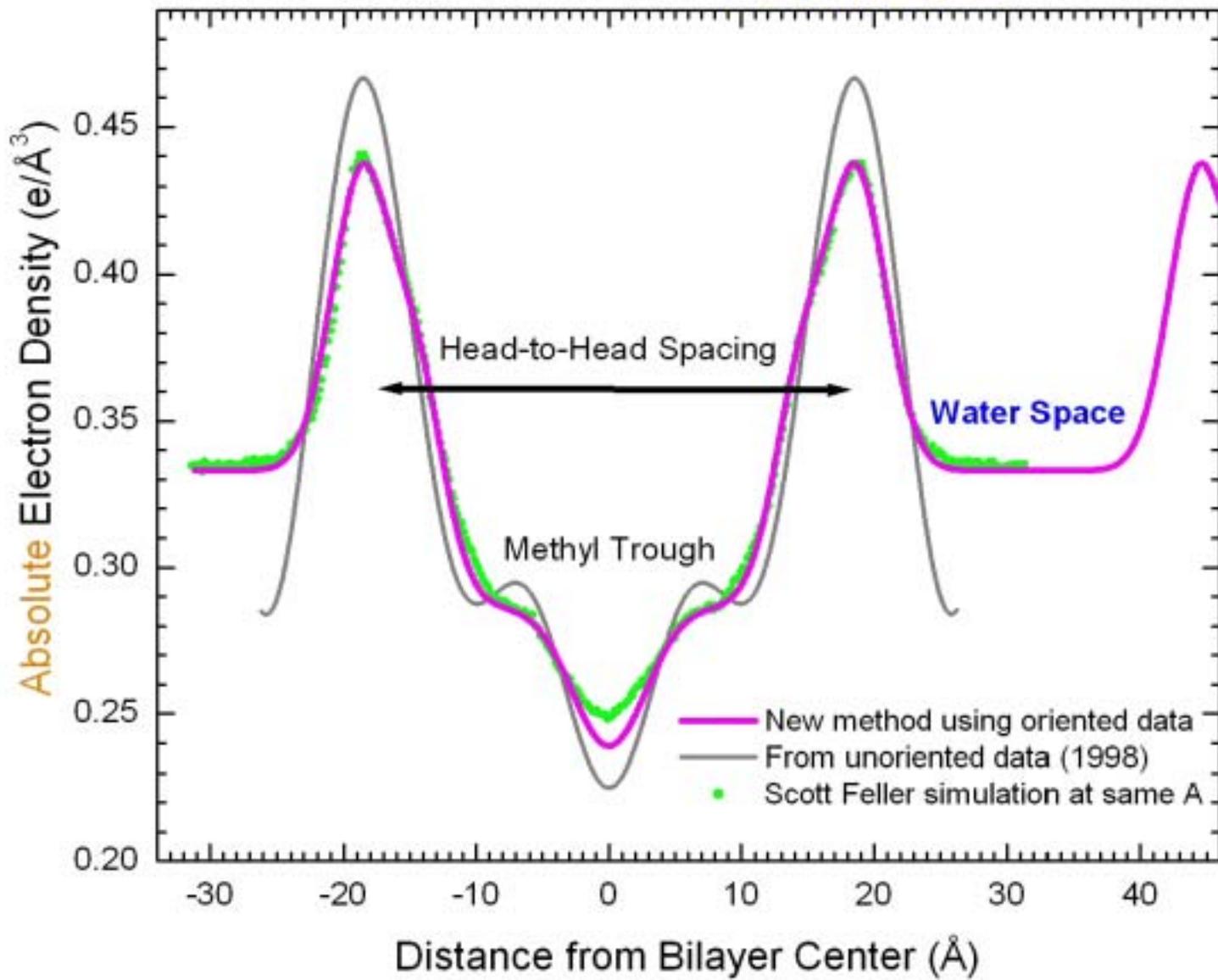
Bootstrap

Strategy for Fluid L_α Phase: Bootstrap from Gel Phase Structure
First done by McIntosh & Simon for DLPE

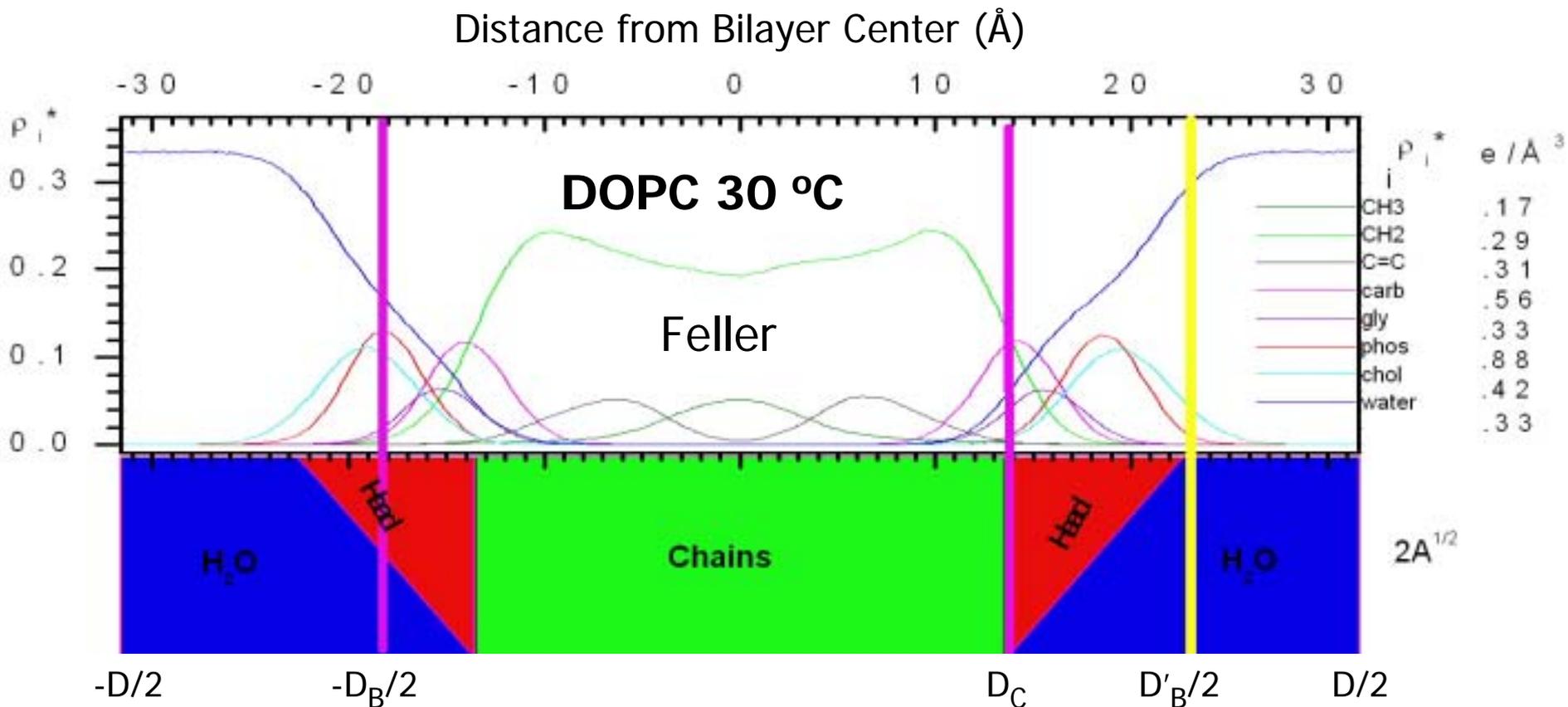
$$A^F = \frac{V^F - V_H^G}{D_C^G - (D_{HH}^G - D_{HH}^F)/2}$$



Electron Density Profiles of Fully Hydrated DOPC



Disorder – First Kind (Guinier)



Conclusions:

1. Have obtained improved **fully hydrated** structure of DOPC and DMPC.
2. Agreement with DOPC simulation performed at same area is outstanding.

<http://lipid.phys.cmu.edu>
For papers and Liu thesis

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John

Yufeng
Liu

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Chu

