

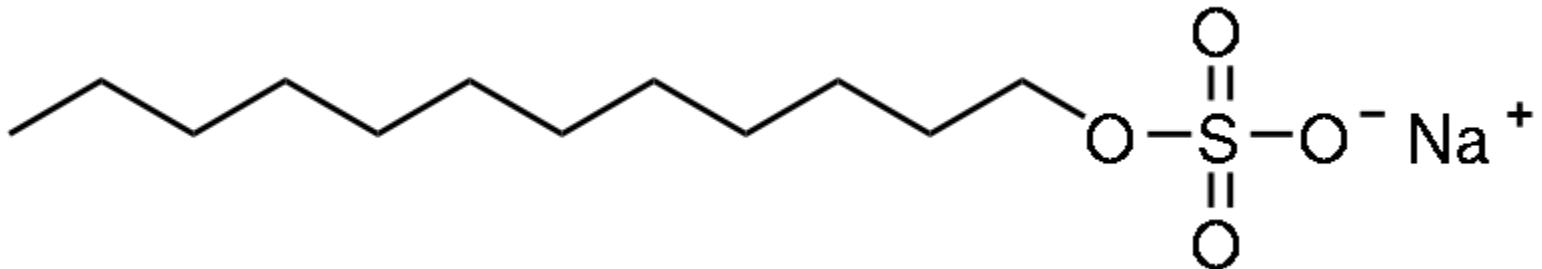
An Investigation of the Phase Behavior of SDS in water using NG3 SANS

Group II – 2012 NCNR Summer School

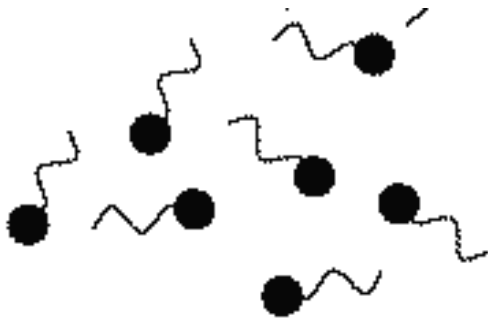
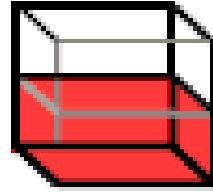
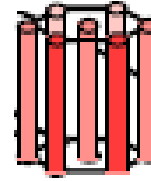
Kiyo Akabori, Greg Barnett, Kiersten
Batzli, Vishal Javvaji, Ricky Lam, Halil
Oztop, Jessie Sun, Charlezetta Wilson

Objectives

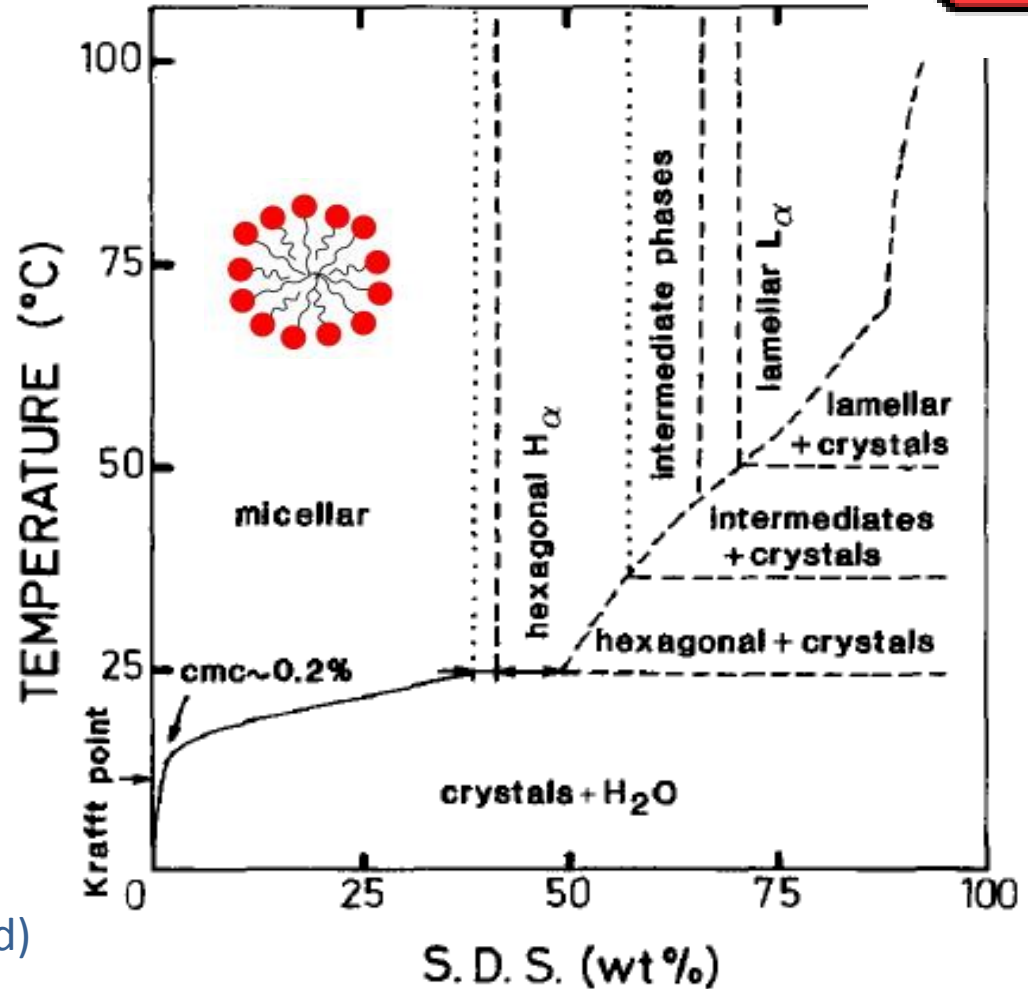
- Hands on experience using Small angle neutron scattering (SANS) @ NG3
- Determine the shape and size of Sodium dodecyl sulfate (SDS) micelles
- Determine the effects of temperature and concentration on the phase behavior of SDS



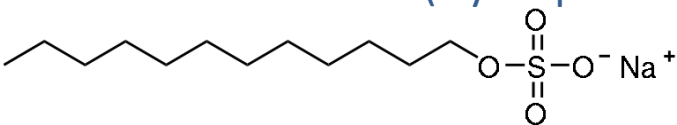
SDS Phase Diagram



Surfactant

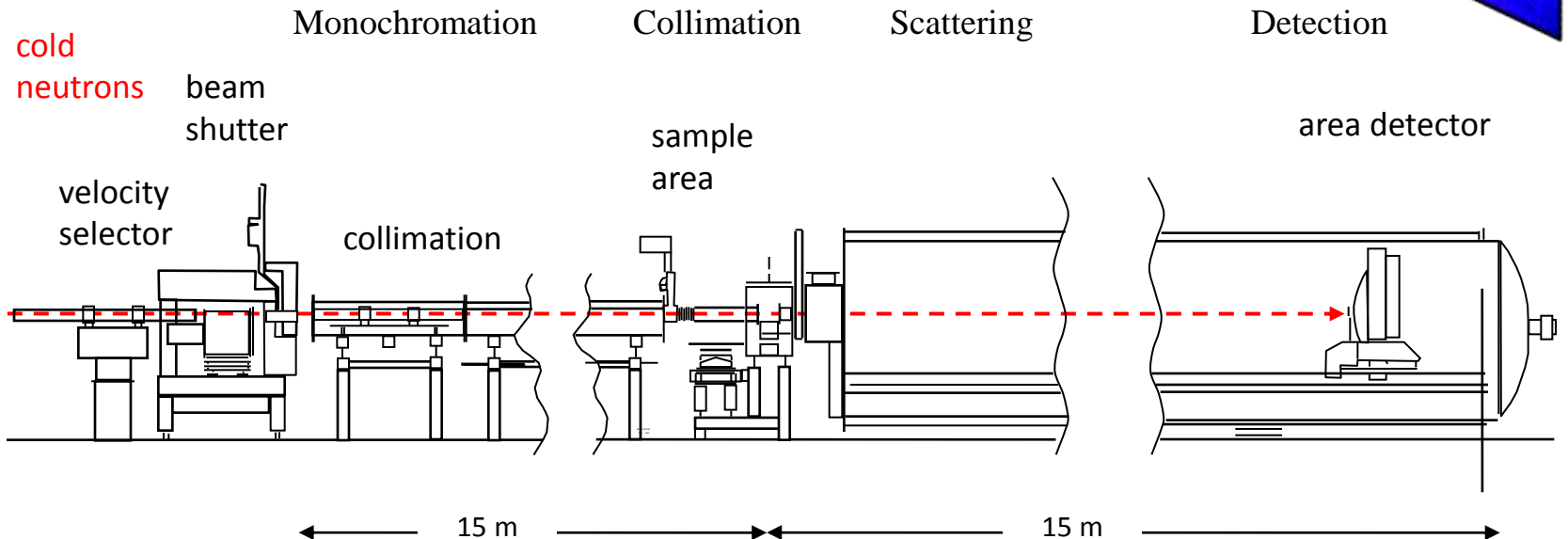
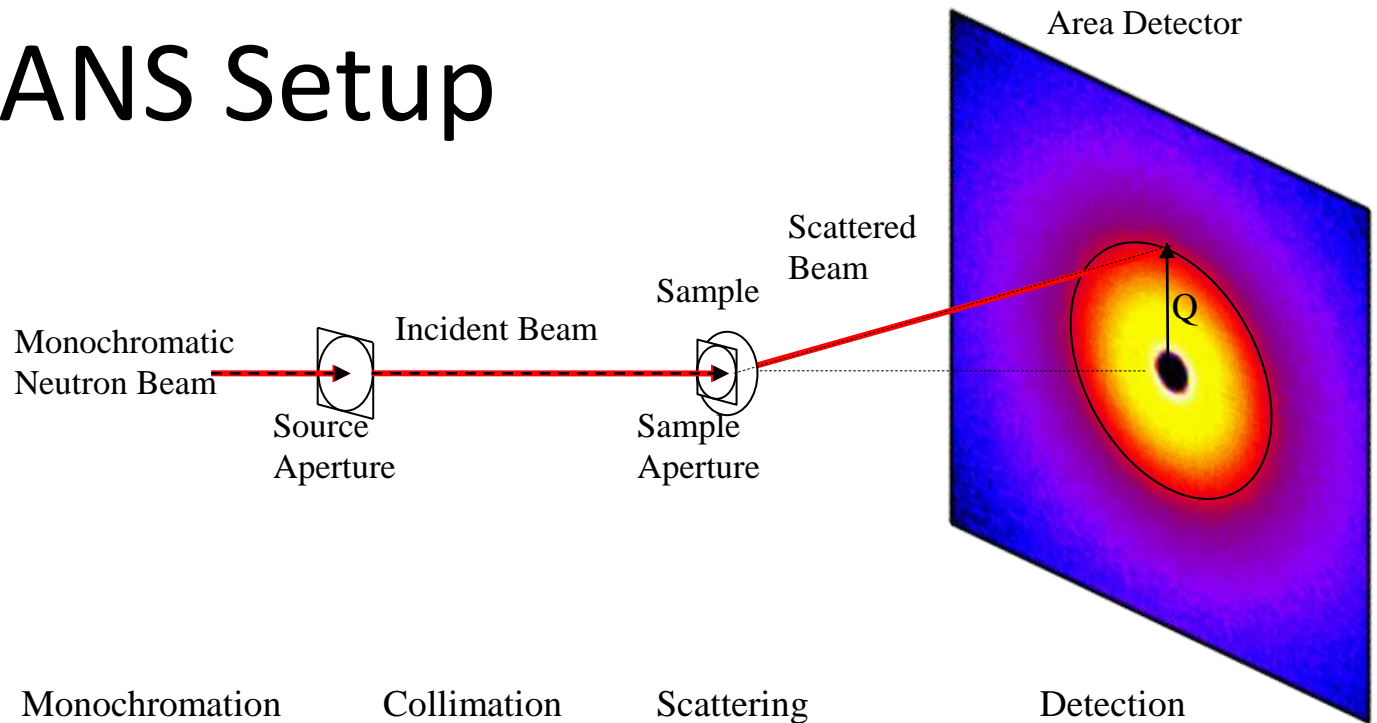


(Hydrophilic Head)



(Hydrophobic Tail)

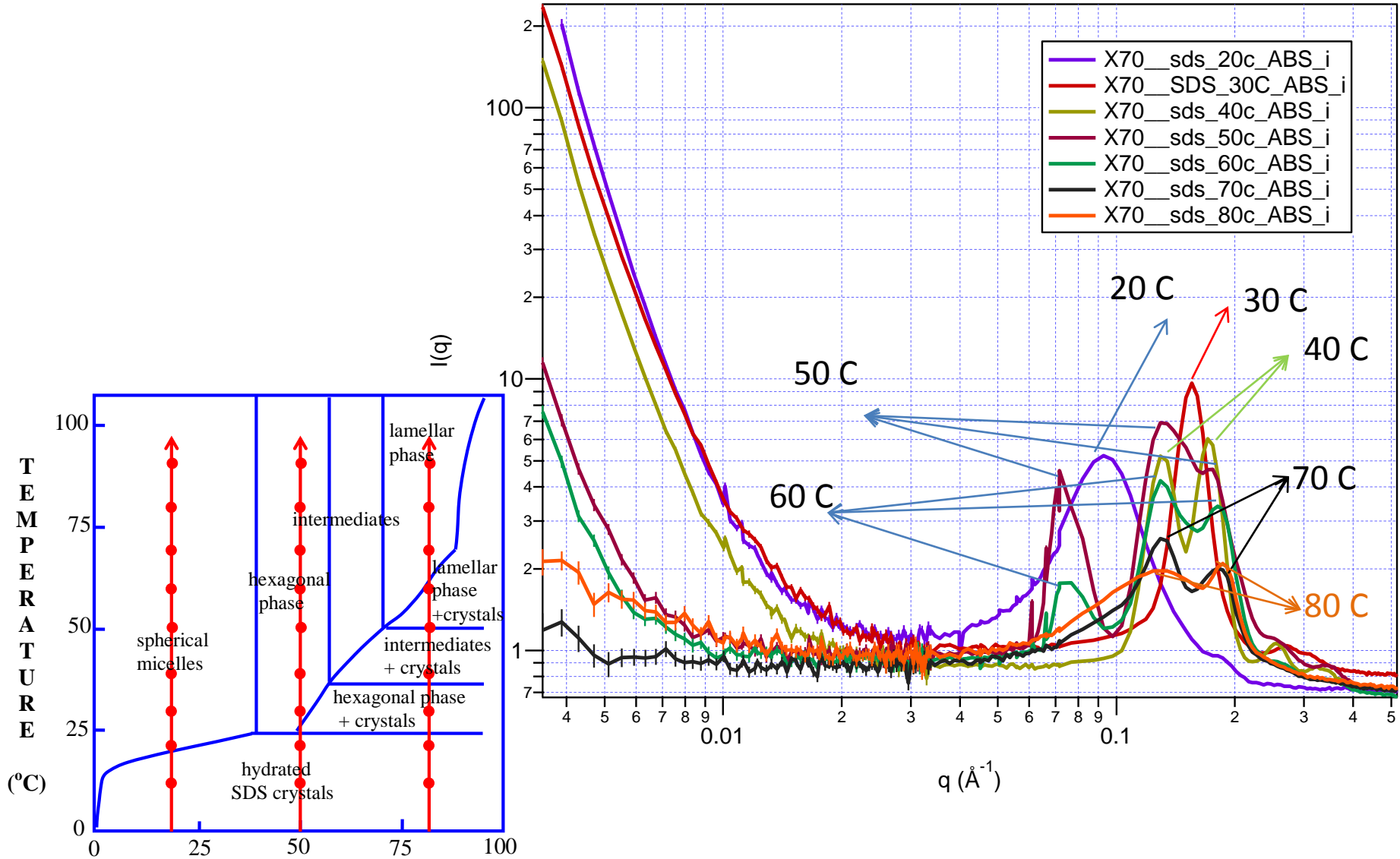
NG3 SANS Setup



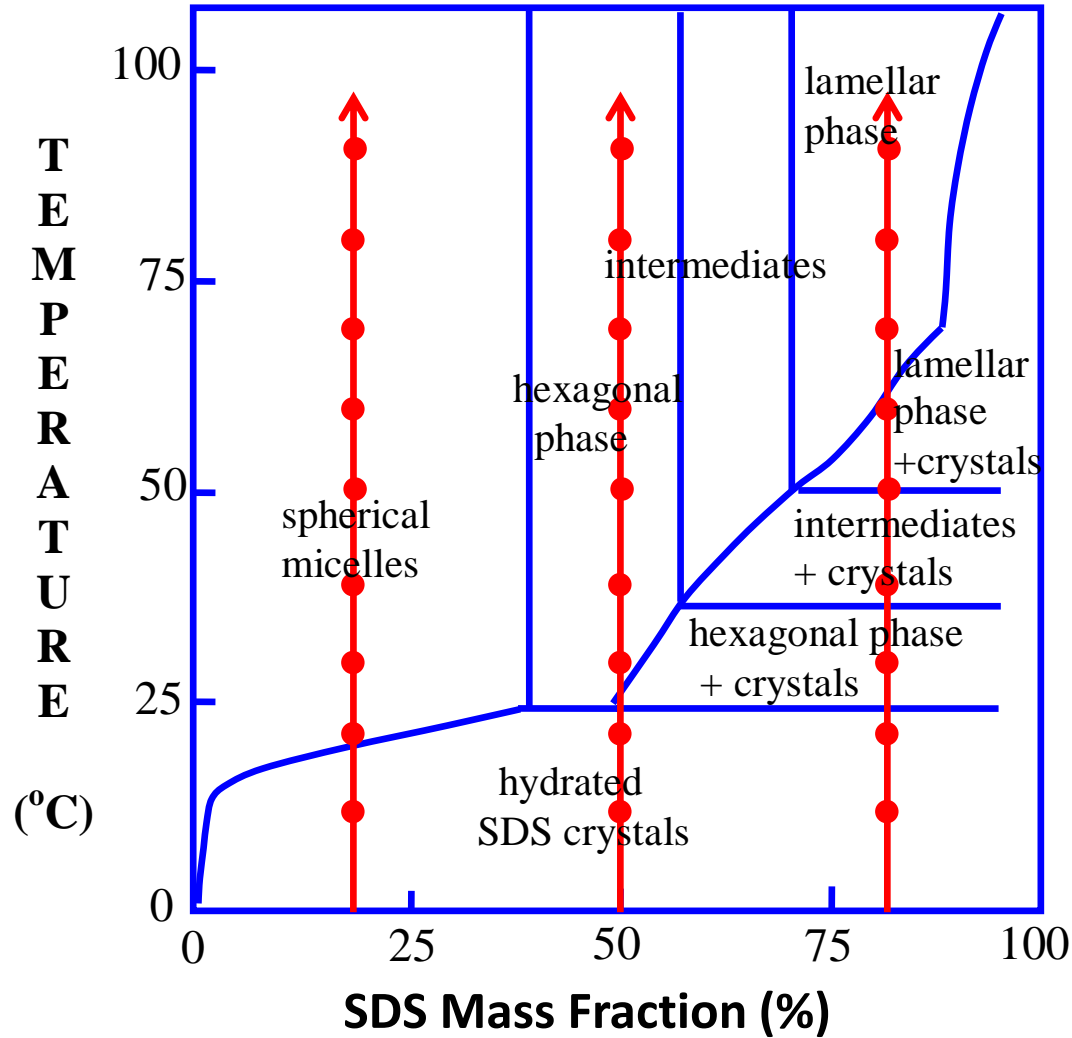
Experimental Design

- SDS micelles were prepared
 - 10wt% to 80wt% in 10wt% increments
- SANS measurements were performed
 - 10°C to 80°C in 10° increments
- Data was analyzed using IGOR
 - NCNR Analysis Macros

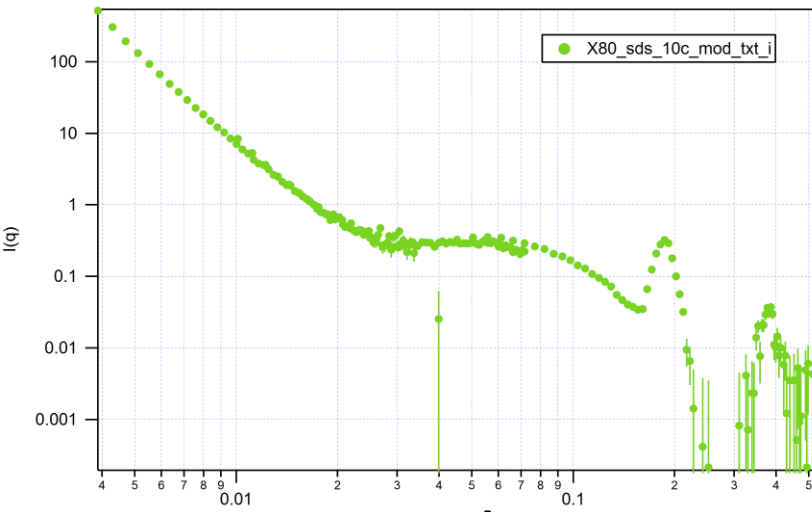
70% SDS Phase Structures



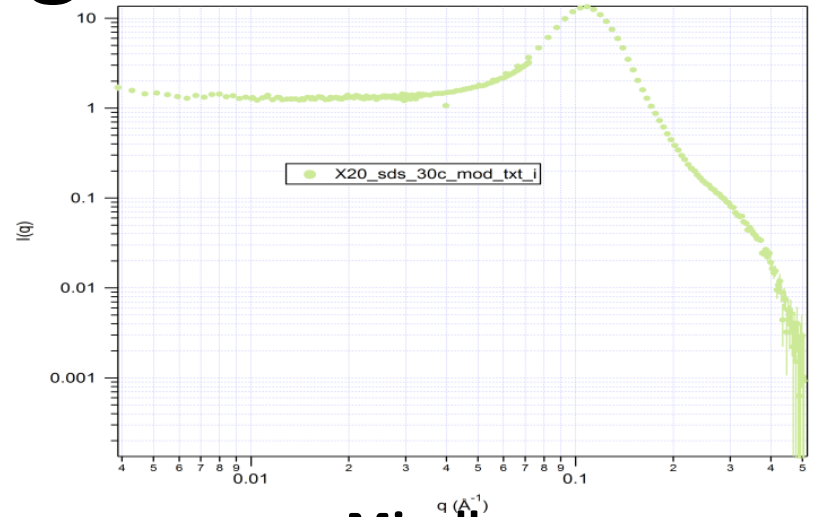
Old Diagram



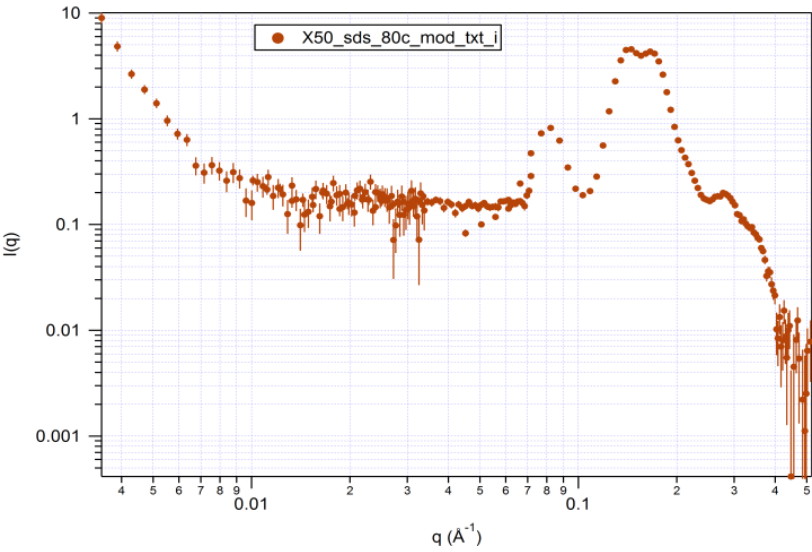
Indexing Peaks



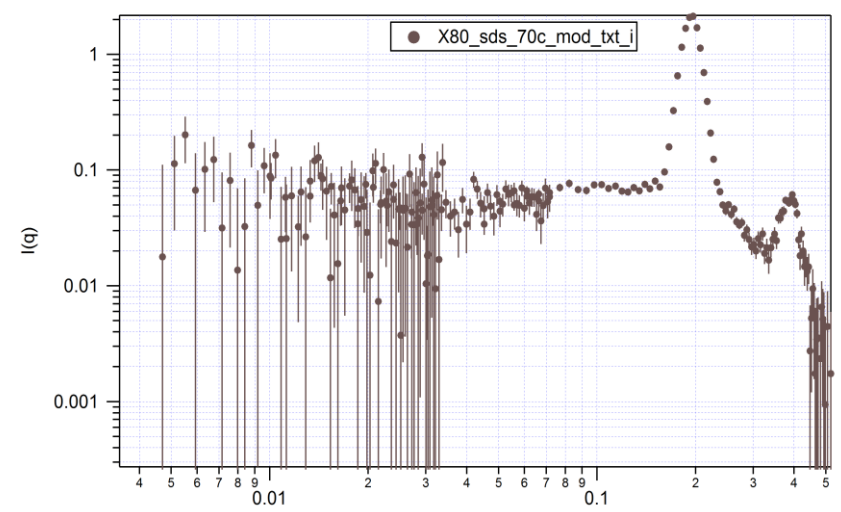
Crystals



Micelles



Hexagonal

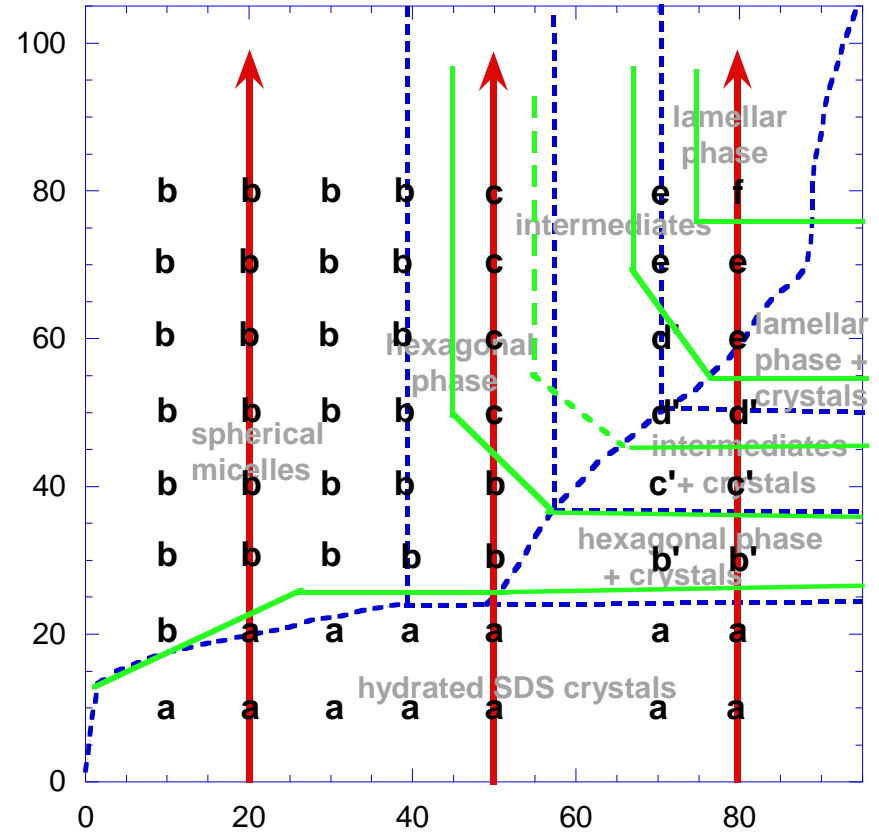
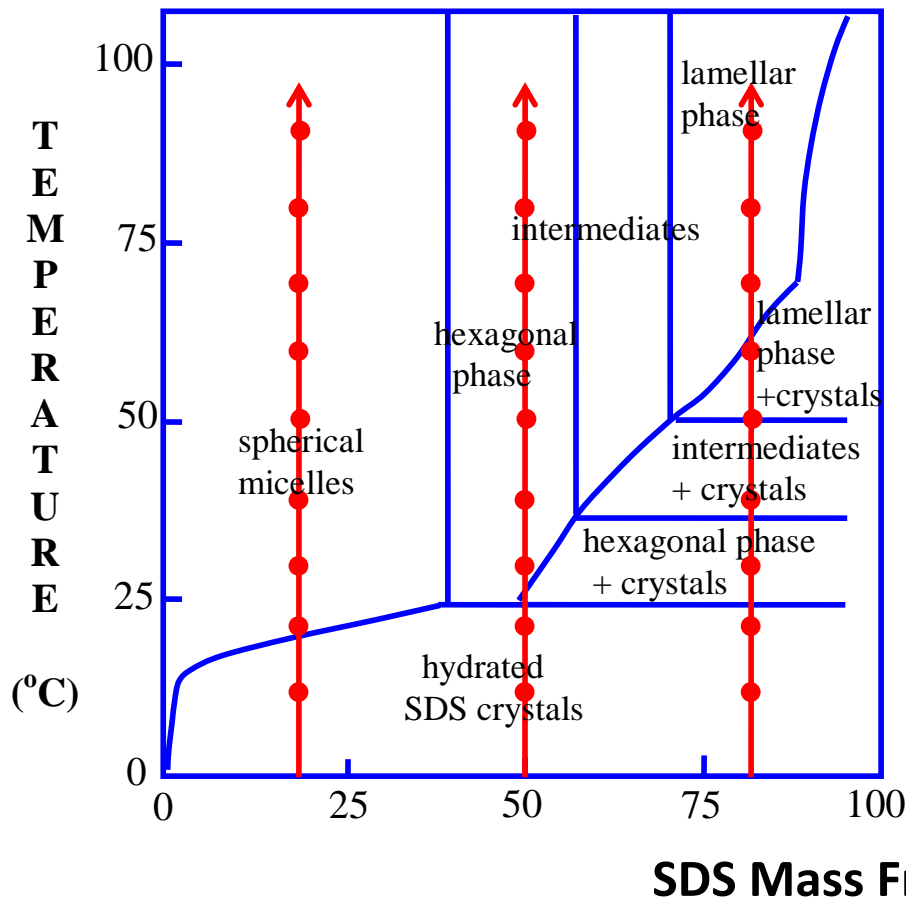


Lamellar

Indexing Peaks

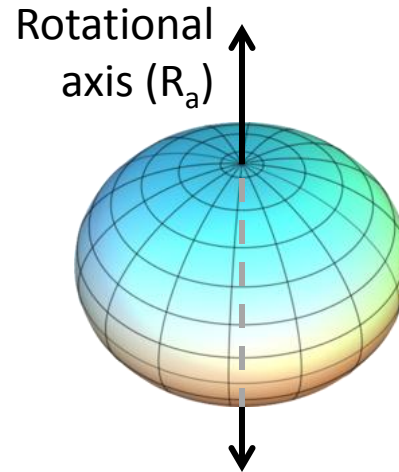
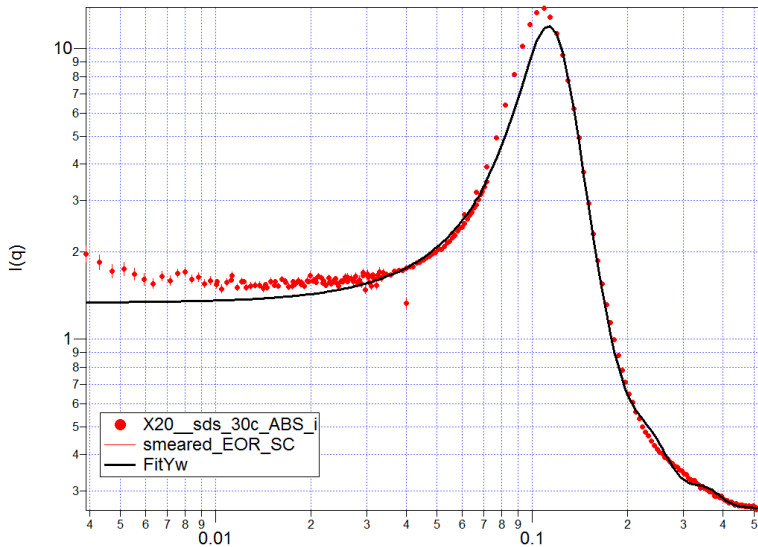
- Structural info
 - Lamellar ($1, \sqrt{4}$)
 - Hexagonal ($1, \sqrt{3}, \sqrt{4}, \sqrt{9}, \sqrt{12}, \dots$)
 - Crystals
- Updating phase diagram accordingly
- Or a combination of structures

Old vs New Phase Diagram



Prolate vs Oblate

Smearred ellipsoid model fit



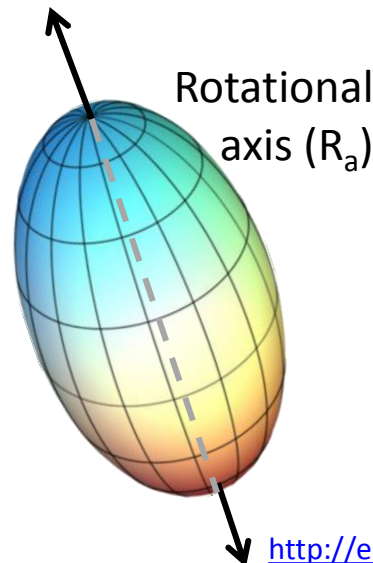
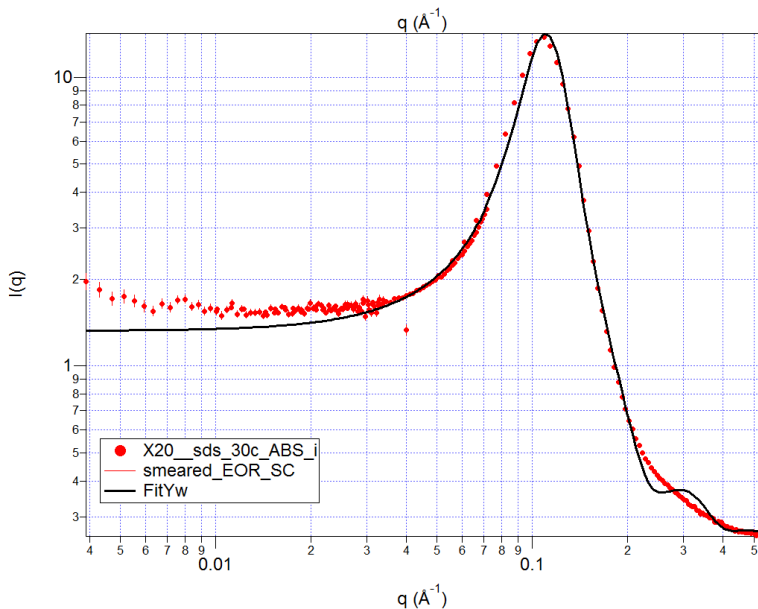
Oblate

$$R_a = 15.1 \text{ \AA}$$

$$R_b = 26.2 \text{ \AA}$$

$$\chi^2 = 6.58$$

<http://en.wikipedia.org/wiki/Spheroid>



Prolate

$$R_a = 36.4 \text{ \AA}$$

$$R_b = 17.7 \text{ \AA}$$

$$\chi^2 = 7.52$$

<http://en.wikipedia.org/wiki/Spheroid>

Radius vs. Temperature

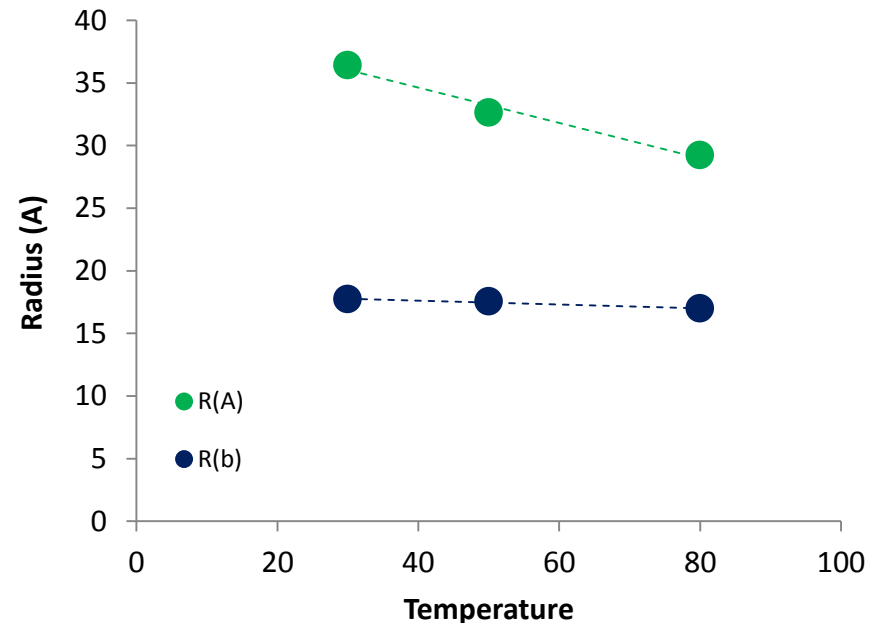
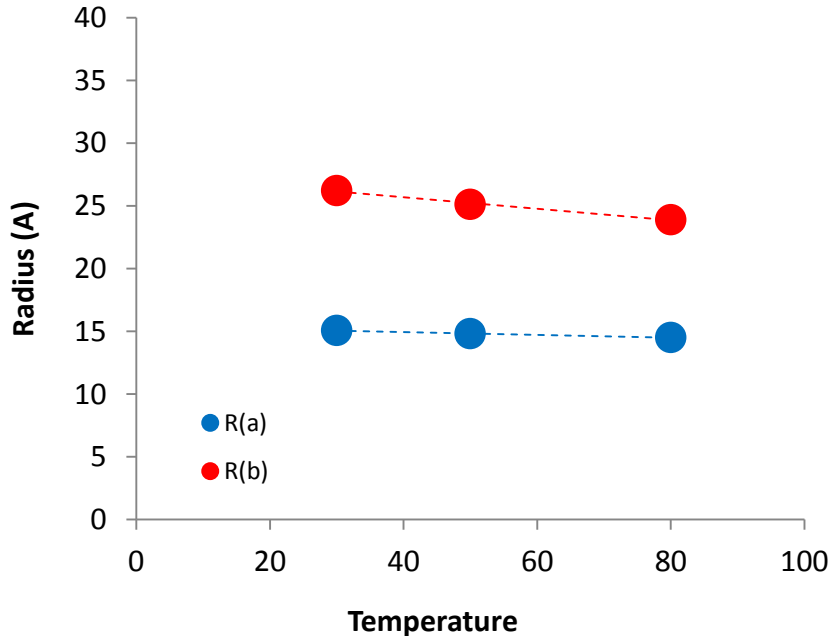
Oblate model (20% mass fraction)

Temp (C)	R_a (Å)	R_b (Å)	χ^2
30	15.0739	26.2076	6.57489
50	14.8203	25.1155	5.40358
80	14.5007	23.8827	3.61079

Prolate model (20% mass fraction)

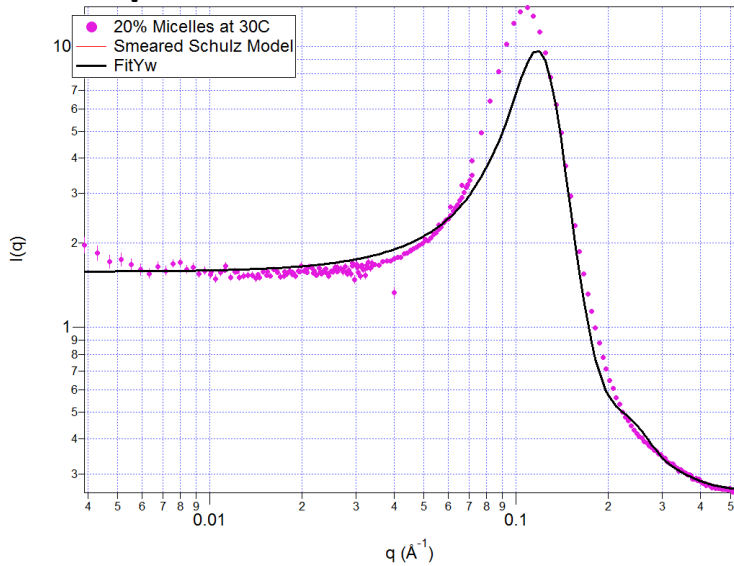
Temp (C)	R_a (Å)	R_b (Å)	χ^2
30	36.3985	17.733	7.51724
50	32.6245	17.5374	7.09351
80	29.2232	16.9808	4.76725

Increasing Temperature = Decreasing Size (both R_a and R_b)

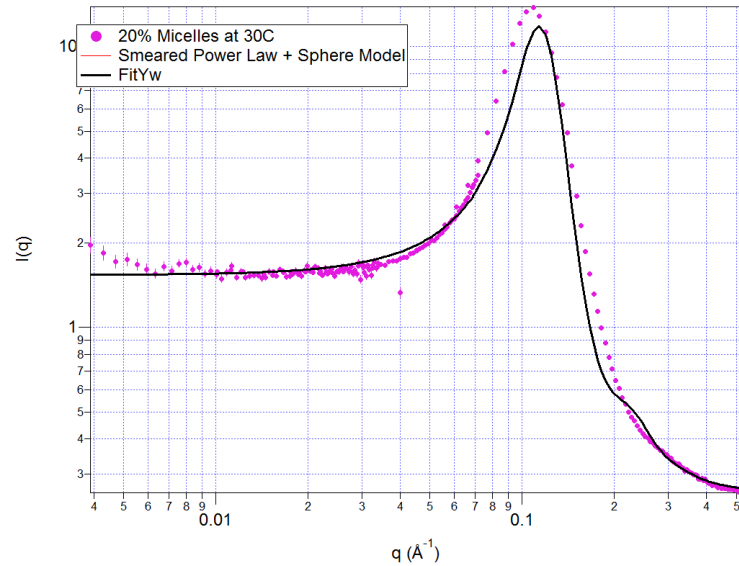


Model Comparison

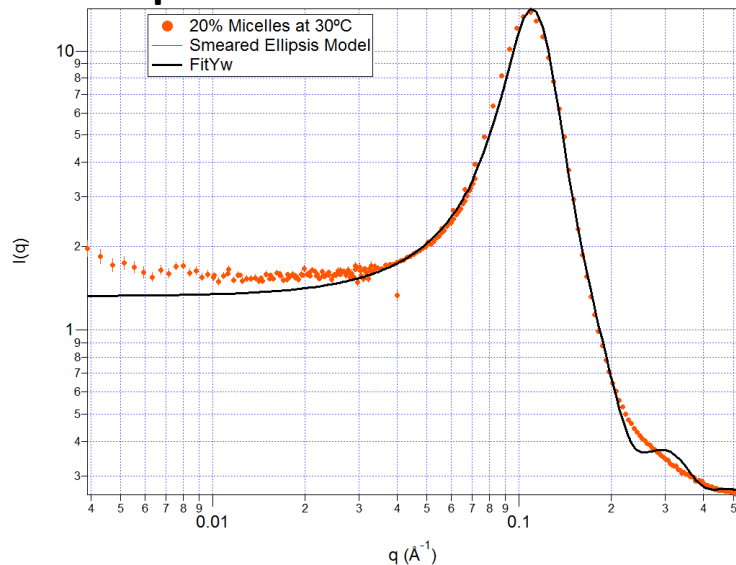
Sphere Model



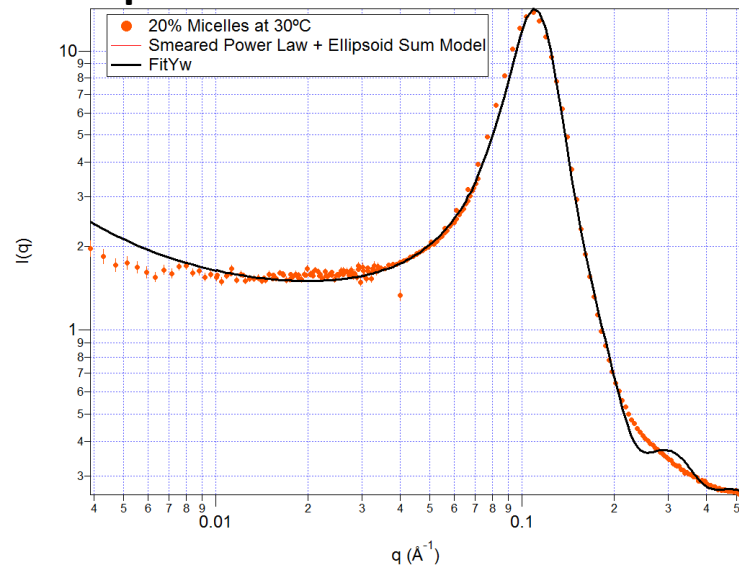
Sphere Model + Power Law Model



Ellipsoid Model

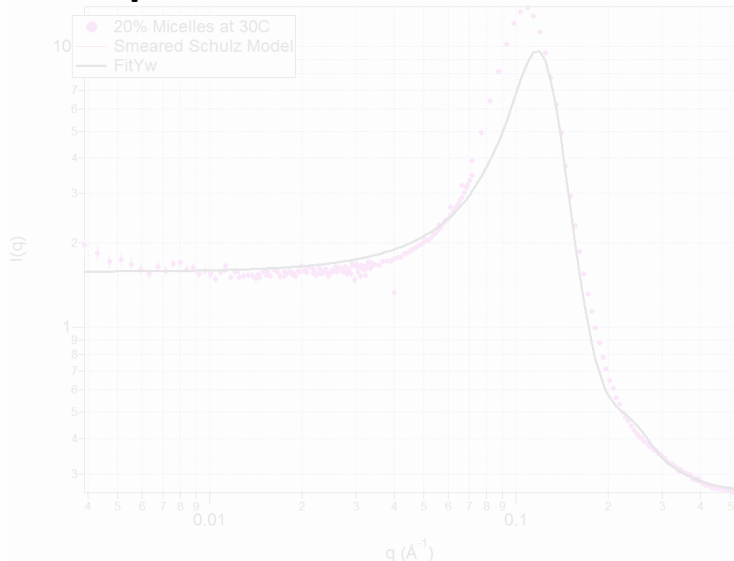


Ellipsoid Model + Power Law Model

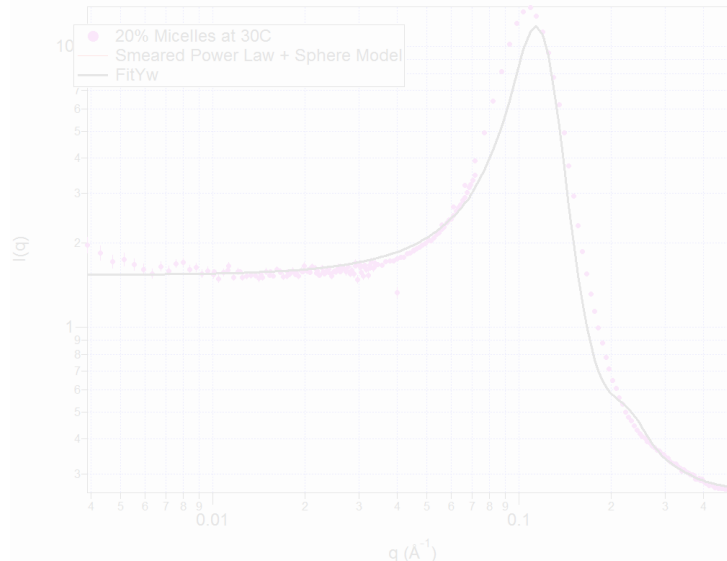


Model Comparison

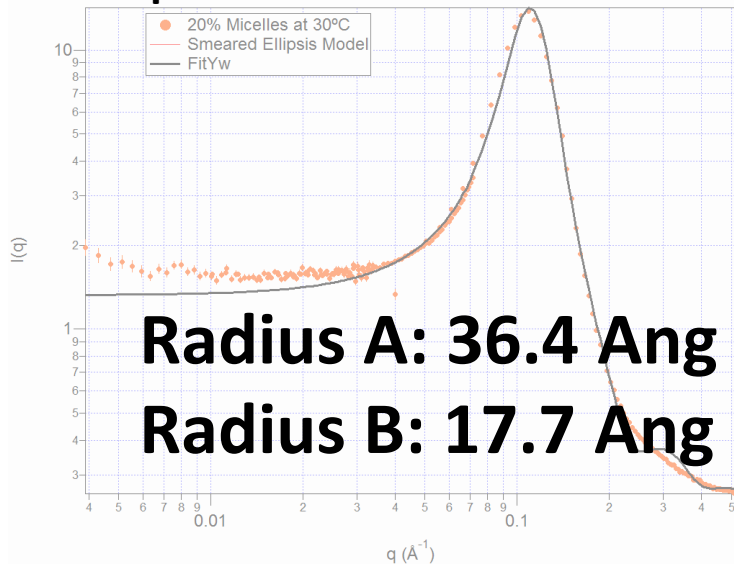
Sphere Model



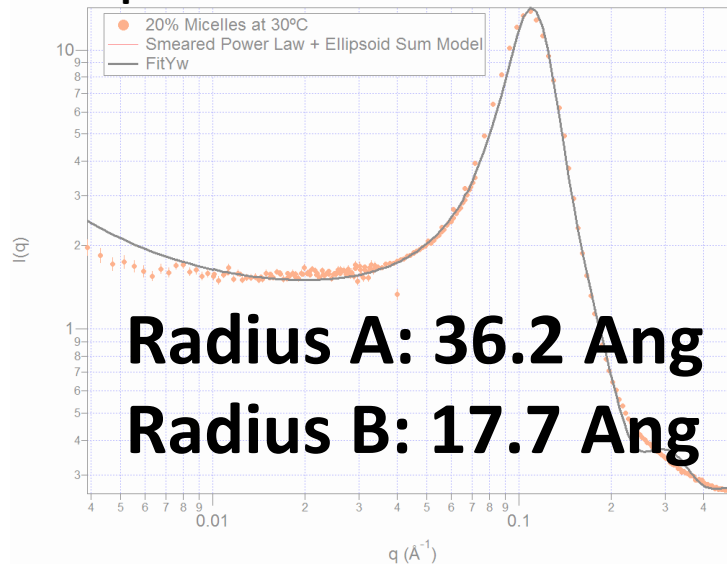
Sphere Model + Power Law Model



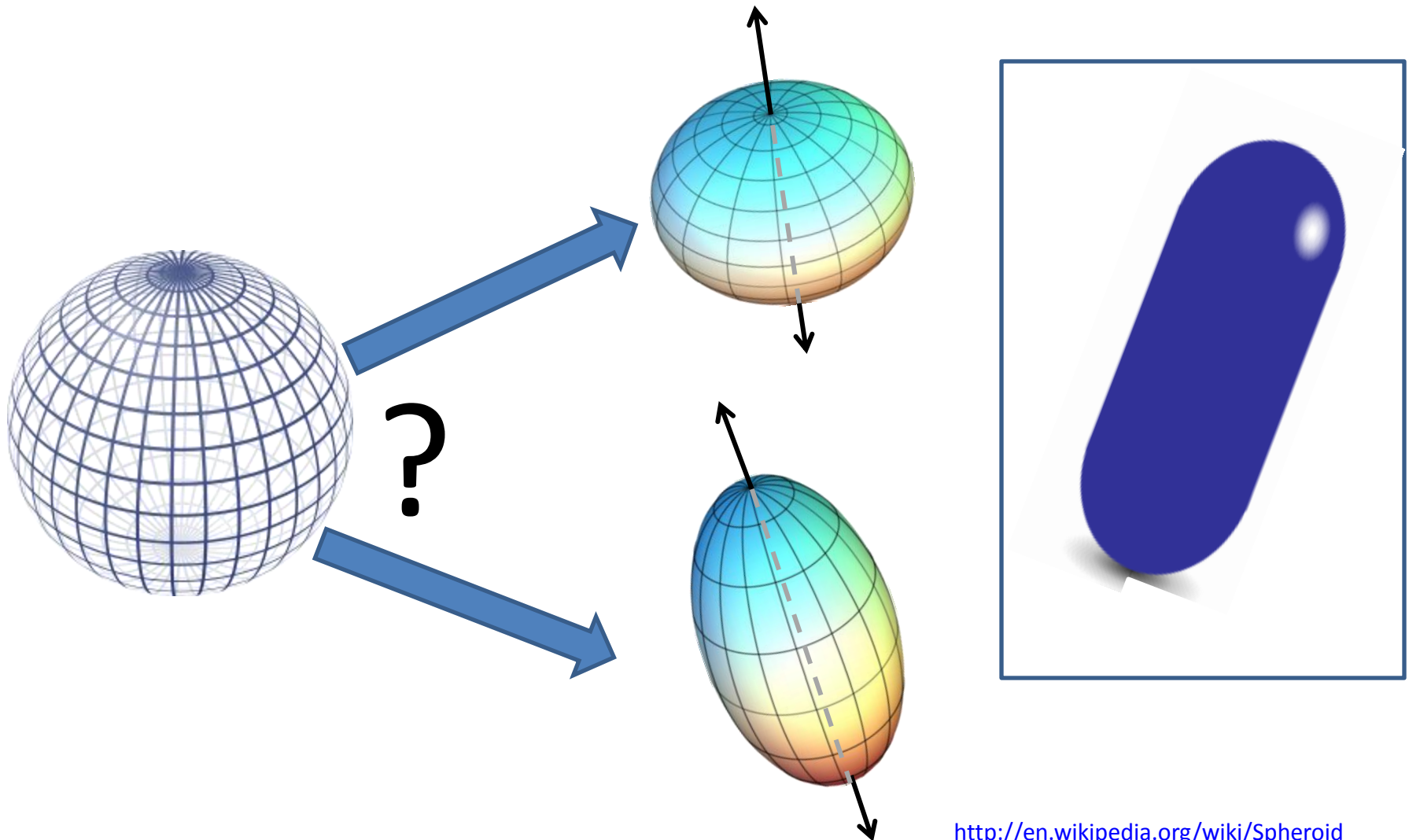
Ellipsoid Model



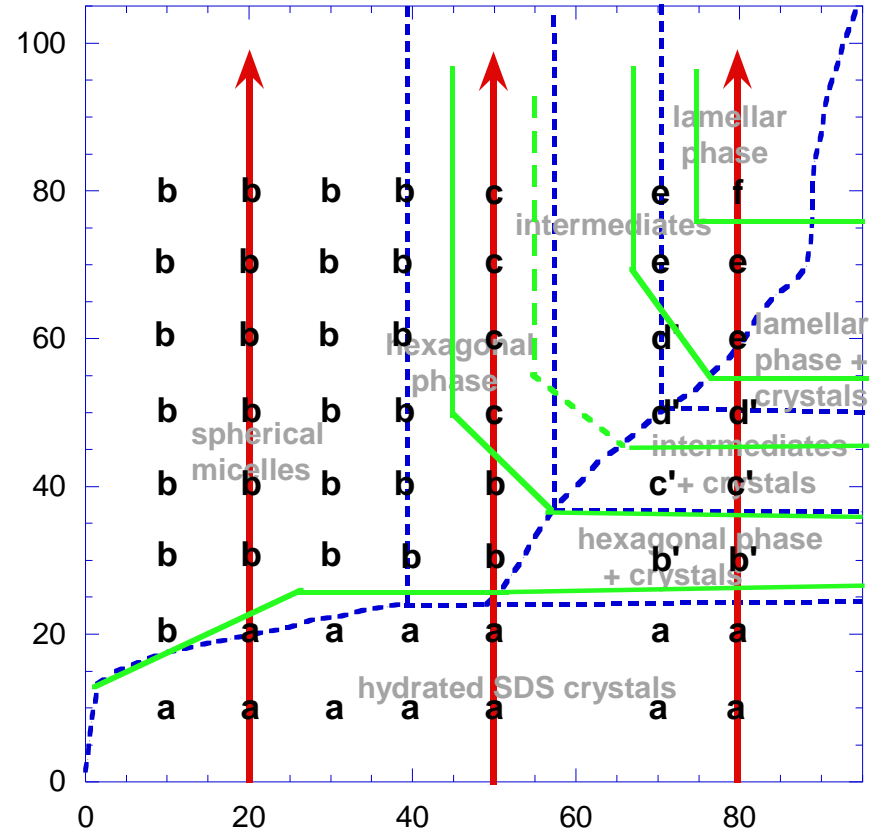
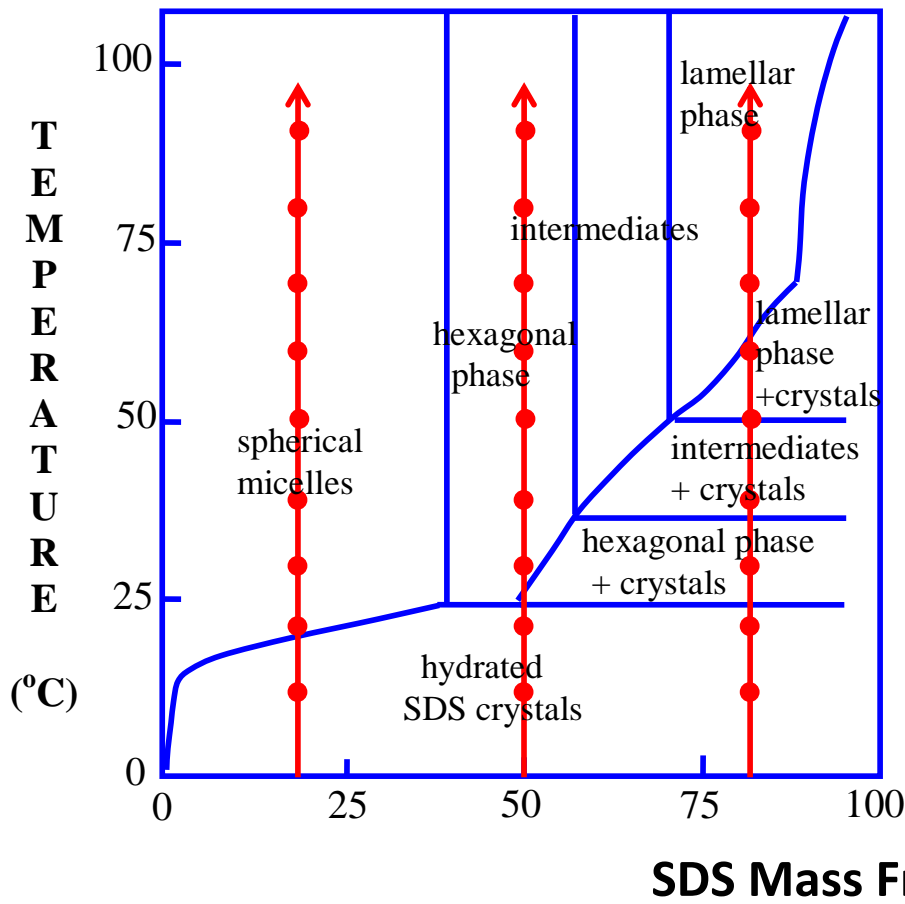
Ellipsoid Model + Power Law Model

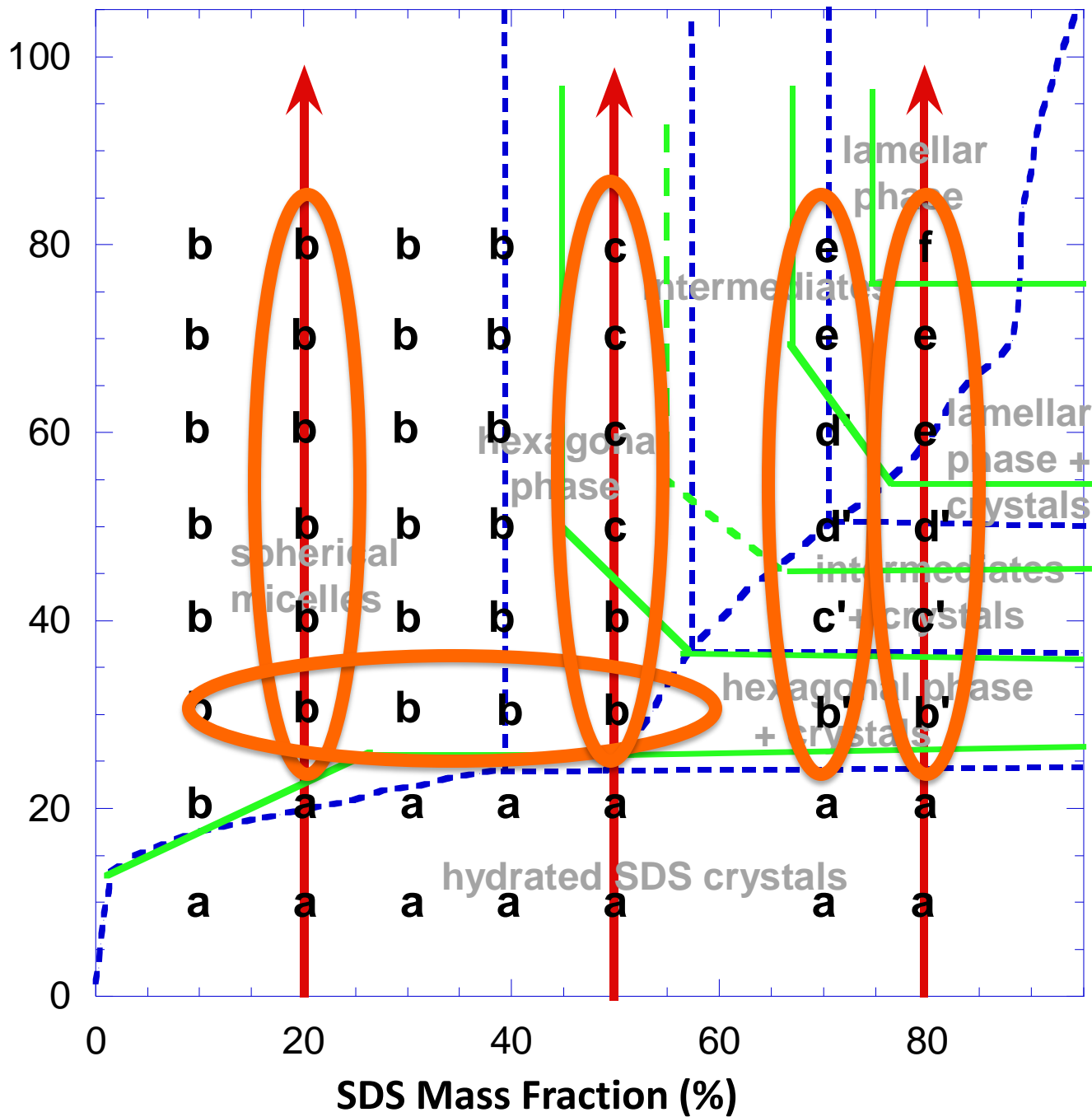


The Great Prolate Oblate State Debate!!



Old vs New Phase Diagram





Summary

- Learned to use SANS to determine structure!!

SDS Micelle Project

- Re-evaluated Phase Diagram
- Prolate vs Oblate?
- Indexed Peaks for micelle structure

- Further Work for Phase Diagram