Web Calculations for SANS

Steve Kline

NCNR Summer School

Neutron Small Angle Scattering and
Reflectometry from Submicron Structures

June 3-7, 2002

Outline

- SLD Calculator
- Scattering Simulator
- Instrument Configurator (SASCALC)

SLD Calculation

- Need all the information possible about the sample
- Stoichiometry
- Mass density (molecular volume)

hPEB	dPMB
C_6H_{12}	$C_5H_{4.5}D_{5.5}$
162 Å^3/molecule	136 Å^3/molecule
84 g/mol	75.5 g/mol
0.86 g/ml	0.92 g/ml

http://www.ncnr.nist.gov/resources/sldcalc.html

SLD Results

hPEB

Compound	C6H12
Density (g/cm^3)	0.86
Wavelength (A)	6
	Calculate
Neutron SLD	-3.07E-7 (A^-2)
Cu Ka SLD	8.34E-6 +9.36E-9i (A^-2
Mo Ka SLD	8.33E-6 +2.08E-9i (A^-2
Neutron Inc. XS	5.93; 33.4 (cm^-1)
Neutron Abs. XS	0.0823 (cm^-1)
Neutron 1/e length	0.166 (cm)

dPMB

Compound	C50H45D55
Density (g/cm^3)	0.92
Wavelength (A)	6
	Calculate
Neutron SLD	3.89E-6 (A^-2)
Cu Ka SLD	8.27E-6 +9.28E-9i (A^-2
Mo Ka SLD	8.26E-6 +2.06E-9i (A^-2
Neutron Inc. XS	2.73; 31.3 (cm^-1)
Neutron Abs. XS	0.037 (cm^-1)
Neutron 1/e length	0.362 (cm)

$b_1 = -4.99 \times 10^{-13}$ cm

$b_1 = 53.3 \times 10^{-13}$ cm

Contrast Factor = $(b_1/V_1 - b_2/V_2)^2 = 1.79 \times 10^{-11}$ Å^{-4}

Calculate Scattering Pattern

- Estimate physical size and shape
- Pick an appropriate model
- Enter all known values
- Guess at the rest

*Rules of Thumb *

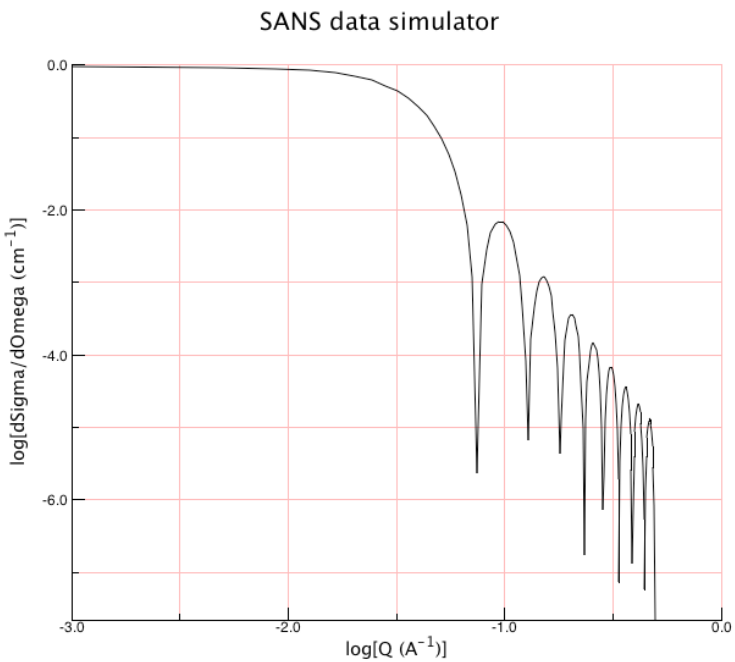
H_2O T(1 mm) = 0.5, $d\Sigma/d\Omega$ = 1 cm^{-1}

D_2O T(1 mm) = 0.9, $d\Sigma/d\Omega$ = 0.06 cm^{-1}

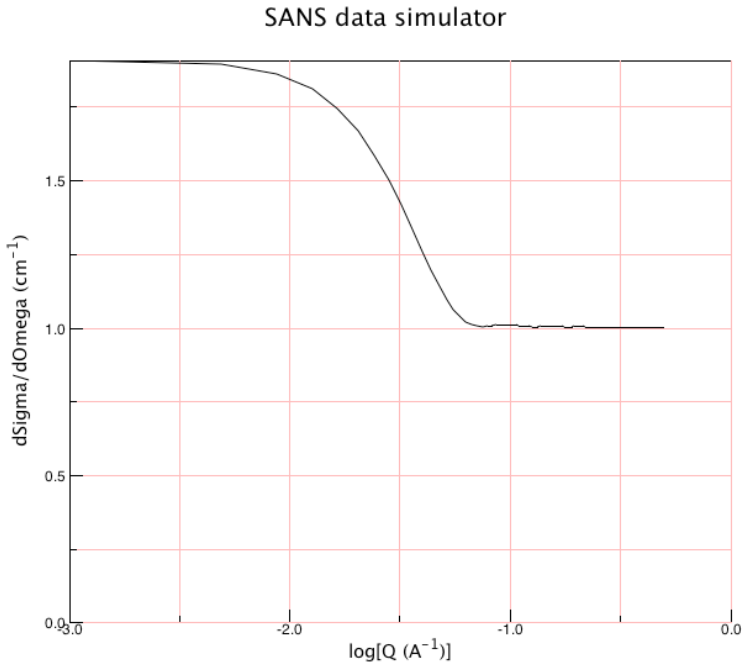
http://www.ncnr.nist.gov/resources/simulator.html

Model Predictions - Simple Sphere

No background



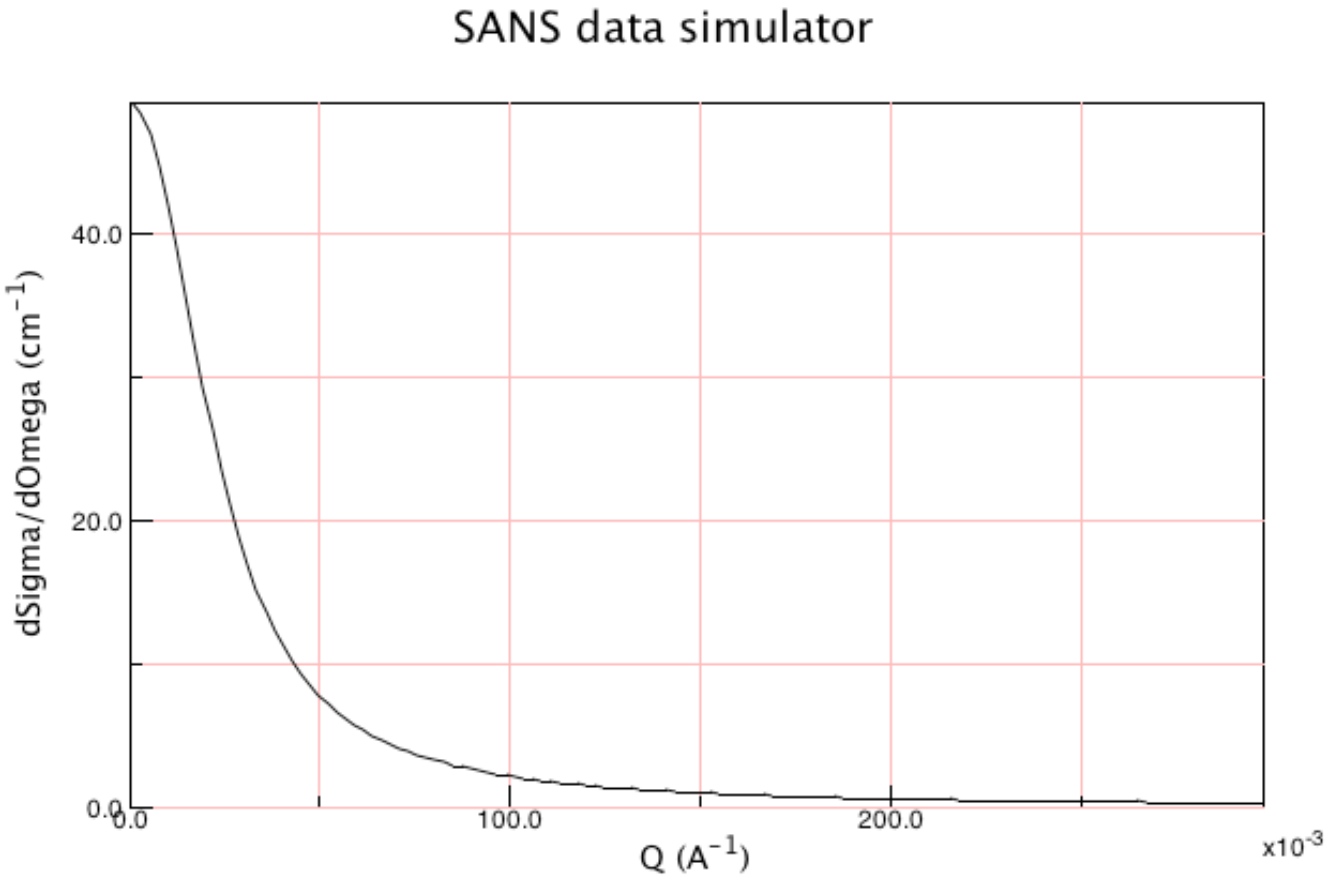
Background = 1 cm^{-1}



Show Data

Sphere		Flat		Log-Log	Smear data?
Scale	1	Vol Fraction (0-1)	0.01	Qmin:	0.001
Radius (A)	60.0			Qmax:	0.5
Contrast (A-2)	1e-6			# Points:	128
Background (cm-1)	0				

RPA Prediction



- Calculated using values in handout
- Background is not very significant

Instrument Configuration

(SASCALC on the VAX)

- Estimate size
- Where in q-space is the scattering happening?

$R_g = \mathrm{sqrt}(Nl^2/6) \sim 100$ Å

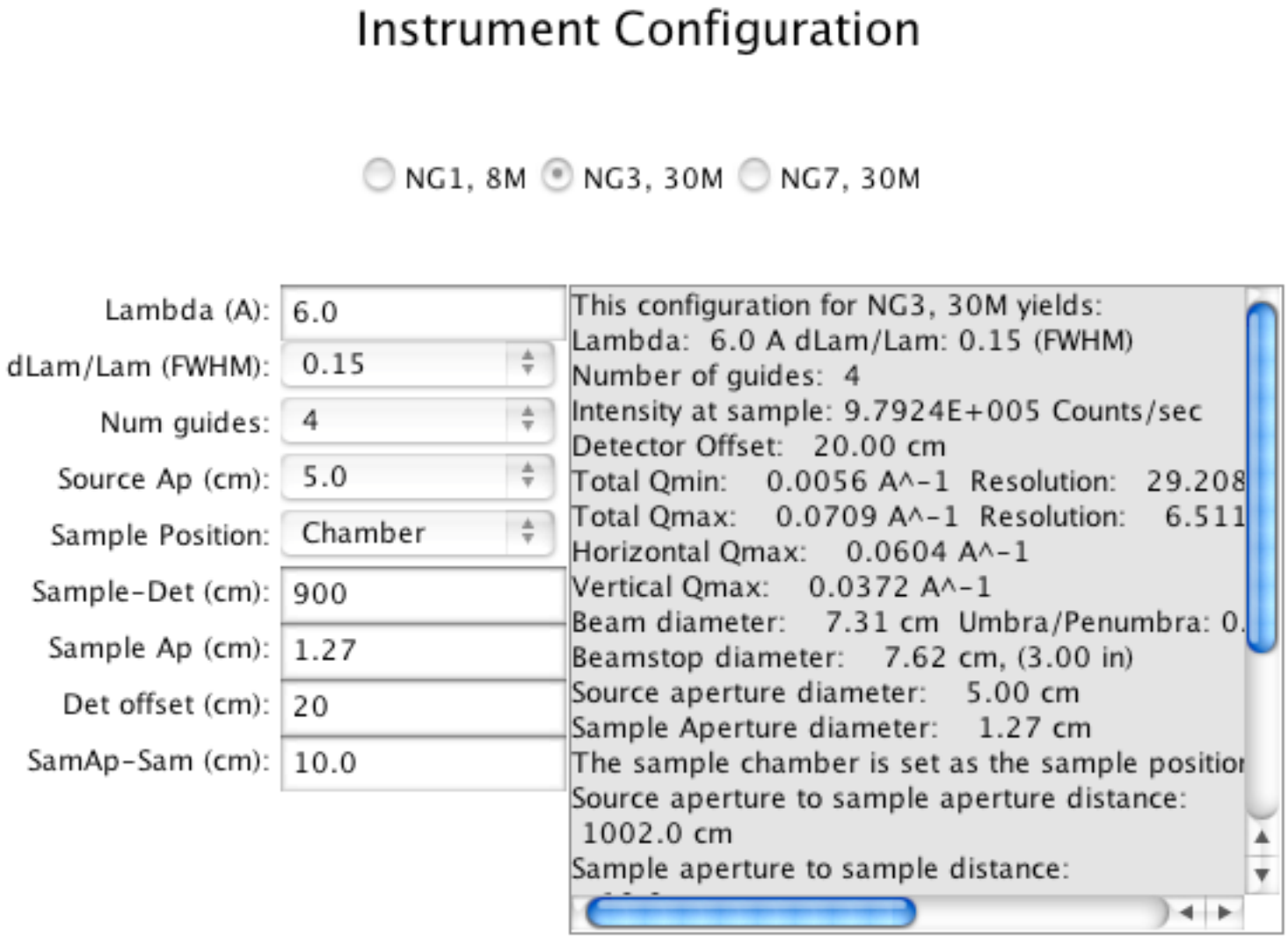
$l \sim 6$ Å

$Q_{min} < 1/R_g \sim 0.01$ Å^{-1}

$Q_{max} > 1/l \sim 0.17$ Å^{-1}

http://www.ncnr.nist.gov/resources/sansplan.html

Instrument Configuration Simulation



Other Tools on the NCNR Website

- Calculation tools http://www.ncnr.nist.gov/resources/index.html
- Nuclear properties http://www.ncnr.nist.gov/resources/n-lengths/
- Manuals http://www.ncnr.nist.gov/programs/sans/manuals/index.html
- Tutorials http://www.ncnr.nist.gov/programs/sans/tutorials/index.html
- Reduction and Analysis http://www.ncnr.nist.gov/programs/sans/manuals/index.html
- Instrument information http://www.ncnr.nist.gov/programs/sans/sans_inst.html
- Available Equipment http://www.ncnr.nist.gov/programs/sans/equipment/index.html
- Access information! http://www.ncnr.nist.gov/access.html
- Proposal information http://www.ncnr.nist.gov/beamtime.html
- Monetary Assistance programs http://www.ncnr.nist.gov/outreach.html
- Summer School notices http://www.ncnr.nist.gov/summerschool/index.html