SANS in McStas

2019 CSNS McStas School

Agenda

- A quick discussion of the SANS technique
- Sample models for SANS in McStas

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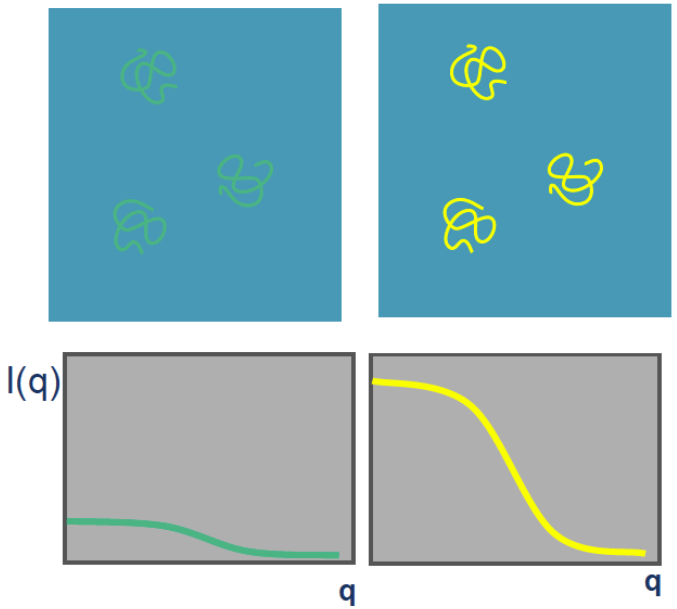
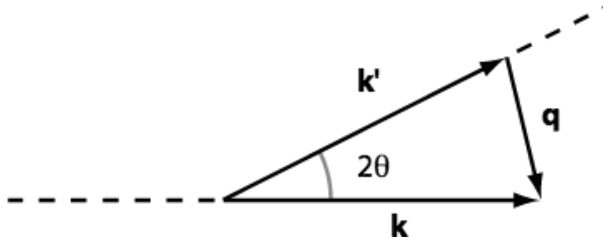
Small angle scattering SANS

- SANS method can be used for many types of material
- Often: Molecule + Liquid (buffer solution)
- Isotropic scattering





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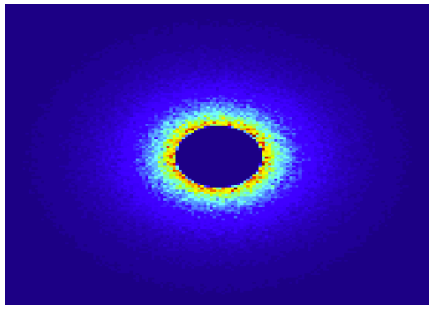
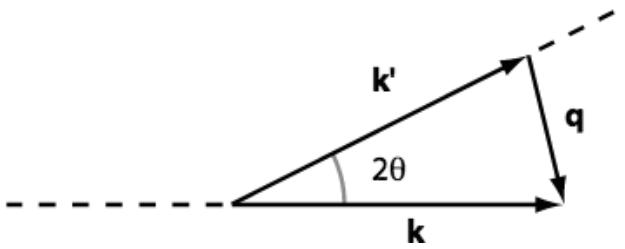
SANS



$$q = \frac{4\pi}{\lambda}\sin(\theta)$$

Small Angle Neutron Scattering

- Elastic Scattering
- Small angle -> small q -> big r
- Gain information on the molecular scale 10-100Å



- Low signal to noise
- Contrast method
- Instrument requirements: good collimation, long flight distance after detector.

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SANS other samples

McStas has a suite of SANS-models:

Try ellipsoidal and

cylindrical particles

-or-

Elliptic cylinders

Go for Nanodiscs and Liposomes

Also – SASmodels from SASview

- SANS_AnySamp.comp
- SANS_DebyeS.comp
- SANSCylinders.comp
- SANSEllipticCylinders.comp
- SANSGuinier.comp
- SANSLiposomes.comp
- SANSNanodiscs.comp
- SANSNanodiscsFast.comp
- SANSNanodiscsWithTags.
- SANSNanodiscsWithTagsFast
- SANSPDB.comp
- SANSPDBFAST.comp
- SANSShells.comp
- SANSSpheres.comp

SANS spheres

Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
R	AA	Radius of scattering hard spheres	100
Phi	1	Particle volume fraction	1e-3
Delta_rho	fm/AA^3	Excess scattering length density	0.6
sigma_abs	m^-1	Absorption cross section density at 2200 m/s	0.05
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert . dimension of sample, as a height for cylinder/box	0
zdepth	m	depth of sample	0
radius	m	Outer radius of sample in (x,z) plane for cylinder/sphere	0
target_x			0
target_y	m	position of target to focus at	0
target_z			6
target_index	1	Relative index of component to focus at, e.g. next is +1	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
focus_r	m	Detector (disk-shaped) radius	0

Dilute, monodisperse, hard spheres in solution, with given contrast and radius

SasView_models

Input parameters

Parameters in **boldface** are required; the others are optional.

Name	Unit	Description	Default
model_index			21
model_scale			1.0
model_pars			{60}
model_abs	1/m	Absorption cross section density at 2200 m/s	0.5
xwidth	m	horiz. dimension of sample, as a width	0
yheight	m	vert . dimension of sample, as a height for cylinder/box	0
zdepth	m	depth of sample	0
radius	m	Outer radius of sample in (x,z) plane for cylinder/sphere	0
target_x	m	relative focus target position	0
target_y	m	relative focus target position	0
target_z	m	relative focus target position	6
target_index	1	Relative index of component to focus at, e.g. next is +1	0
focus_xw	m	horiz. dimension of a rectangular area	0
focus_yh	m	vert. dimension of a rectangular area	0
focus_aw	deg	horiz. angular dimension of a rectangular area	0
focus_ah	deg	vert. angular dimension of a rectangular area	0
focus_r	m	Detector (disk-shaped) radius	0

SasView_models

47	parallelepiped	(sld, solvent_sld, a_side, b_side, c_side)
48	parallelepiped_xy	(sld, solvent_sld, a_side, b_side, c_side, theta, phi, psi)
49	pearl_necklace	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_sld, solvent_sld)
50	pearl_necklace_xy	(radius, edge_separation, string_thickness, number_of_pearls, sld, string_sld, solvent_sld)
51	sphere	(sld, solvent_sld, radius)
52	sphere_xy	(sld, solvent_sld, radius)
53	star_polymer	(radius2, arms)
54	star_polymer_xy	(radius2, arms)
55	stickyhardsphere	(effect_radius, volfraction, perturb, stickiness)
56	stickyhardsphere_xy	(effect_radius, volfraction, perturb, stickiness)
57	triaxial_ellipsoid	(sld, solvent_sld, req_minor, req_major, rpolar)
58	triaxial_ellipsoid_xy	(sld, solvent_sld, req_minor, req_major, rpolar, theta, phi, psi)

First exercise will take place on the e-neutrons.org infrastructure (using a web-simulator)

1. Please fill in the form at https://www.e-neutrons.org/?page_id=423
2. (Once everyone has done this, I will enable the accounts)
3. You will receive an email with login-credentials
4. Use these credentials to log in to the simulation quiz at https://www.e-neutrons.org/moodle/mod/quiz/view.php?id=4276
5. Follow the instructions in the quiz

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