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6 SEPTEMBER 2016
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AINSE
Neutron Small Angle Scattering
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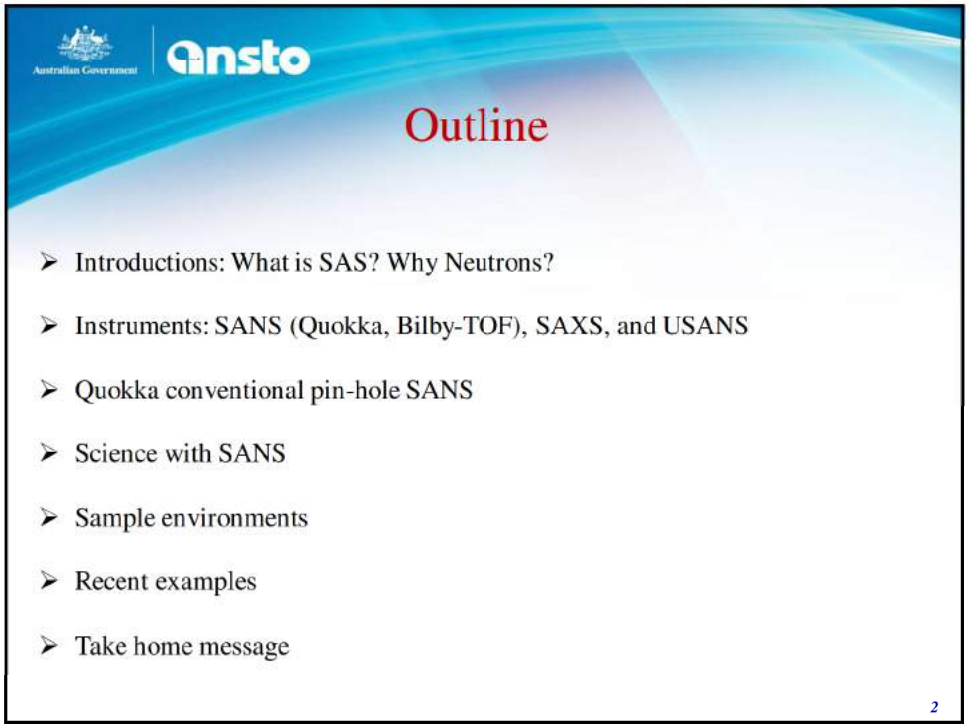
6th September 2016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Outline
Introductions: What is SAS? Why Neutrons?
Instruments: SANS (Quokka, Bilby-TOF), SAXS, and USANS
Quokka conventional pin-hole SANS
Science with SANS
Sample environments
Recent examples
Take home message
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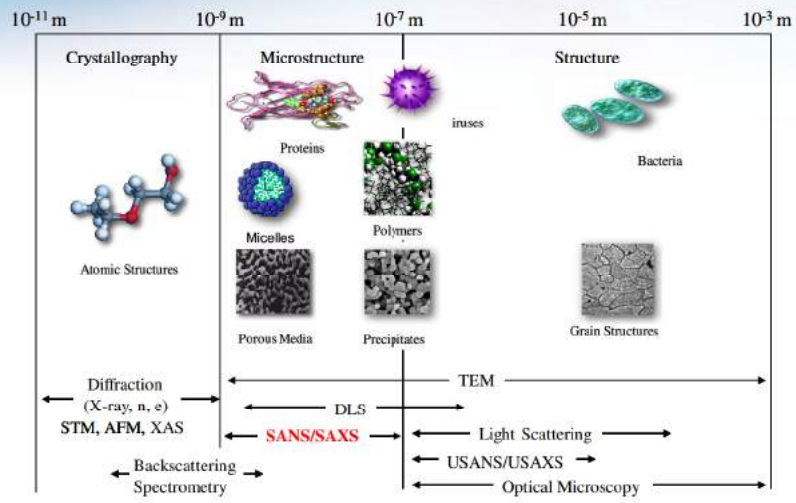
Overview



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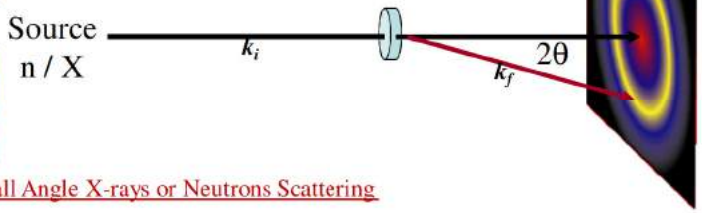
What is Small-Angle Scattering ?

$$q = k_f - k_i = (4\pi/\lambda)\sin\theta$$



Small Angle X-rays or Neutrons Scattering

- X-rays: High intensity, fast (or local), contrast issue.
- Neutrons: Multiple contrast options, labelling, limited availability.
- Size probed inversely proportional to angle.
  - Small angle → small q → large distances

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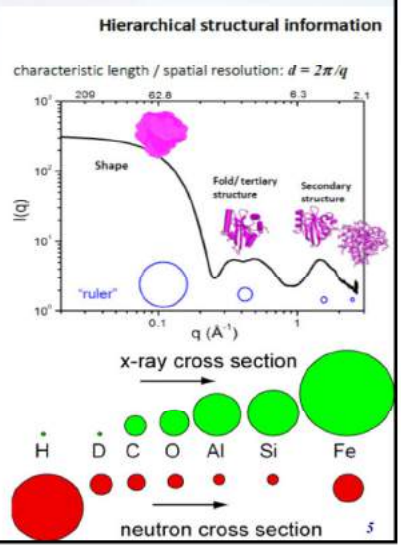
Why Neutrons?

- Neutrons have zero charge and negligible electric dipole → interact with matter via nuclear forces.
- Nuclear forces are very short range.
- Highly penetrating.
- Attenuation of low energy neutrons by Al is ~1%/mm compared to >99%/mm for x-rays.
- Different interaction – "sees" different things
- Non-destructive



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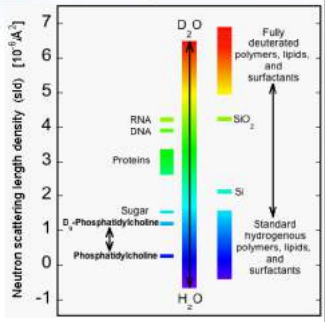
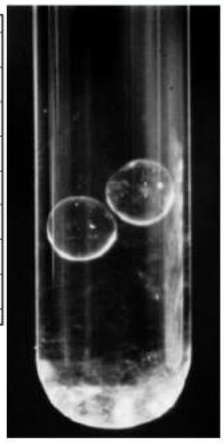
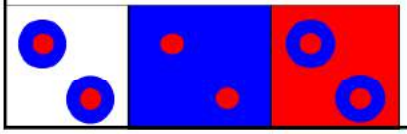
Contrast Variation

- Neutron scattering: Contrast Variation
  - protein – lipid
  - Solute – surfactant
  - protein – sugar
  - solute-solvent
  - part of molecules







G.D. Wignall, Physical properties of polymers, 1993, 424-502. 6

SAS Instruments @ ACNS

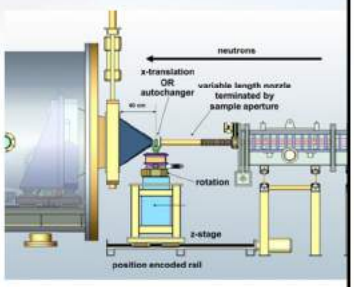
Quokka

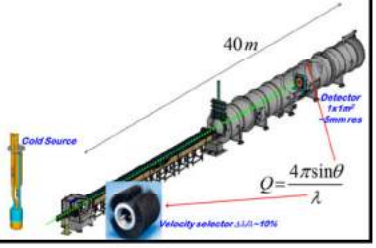
Bilby

Kookaburra

Quokka

- Quokka* is a pin-hole SANS instrument
- Located on the cold guide (CG1) at OPAL
- Q range from 6 x 10^{-4} $Å^{-1}$ to greater than 0.7 $Å^{-1}$
- MgF_2-Focussing optics
- Estimated maximum flux on sample is > 2 X10^7 n/cm^2/s
- Astrium velocity selectors: 7 - 18% resolution
- Pre-sample collimation system: neutron guides and apertures
- Ordela 2D position sensitive detector (1 m^2 area and 5 mm each pixel resolution)





* E.P. Gilbert, J.C. Schulz and Terry J. Noakes, "Quokka" - the Small-Angle Neutron Scattering Instrument at OPAL., Physica B, 385-386 (2006) 1180-1182.

Science with SANS

- Becomes an all-purpose structural tool
- Characterizes a variety of samples:
  - Polymers, food, proteins, metals, ceramics, rocks, magnetic clusters, superconductors etc.
  - Part of molecule/system, multicomponent systems, aggregation etc.
- Complementary to electron microscopy
- SANS can provide particle sizes, shapes, and interaction
- Studies molecules under most relevant conditions
- Requires relative smaller amount of sample
- Fast data acquisition and analysis

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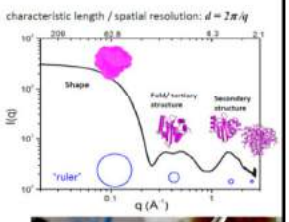
The Basic Scattering Equation

For an ensemble of identical, randomly oriented particles, the intensity of coherently, elastically scattered radiation is dependant only upon the magnitude of q, and can be expressed as:

$$I(q) = N\left(\Delta\overline{\rho}V\right)^2 P(q)S(q)$$



N = molecules/unit volume

V = molecular volume

$\Delta\overline{\rho} = \langle\rho(\mathbf{r})\rangle - \overline{\rho}_s$ = contrast, the scattering density difference between the scattering particle and solvent

$P(q)$ = form factor ⇒ particle shape

$S(q)$ = structure factor ⇒ inter-particle correlation distances

http://gr5.org/index_of_refraction/

Sample Environments

- Two automatic temperature-controlled sample changers: -40 to 120 °C or between room temperature and 250 °C
- New 12 position individual temperature controlled sample changer
- Superconducting magnet up to 11 T and temperatures of <1 K
- A BioLogic SFM-300 stopped flow cell
- Rheo-SANS setup
- 5 position rotating sample changer
- Various sample holders for different applications
- A Rapid Heat Quench Cell: For thermal shock studies
- The neutron Rapid Visco Analyser (nRVA)
- High pressure SANS cell
- In-situ Differential Scanning Calorimetry (DSC)

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Recent Examples

Effects of Crowding and Environment on the Intrinsically Disordered Protein, Rec1-Resilin*

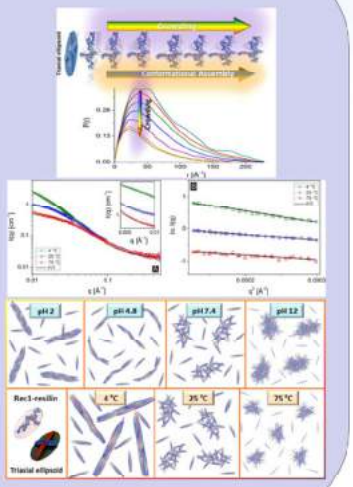
The structural ensembles and transitions of a biomimetic, multi-stimuli-responsive, intrinsically disordered protein (IDP), Rec1-resilin with change in molecular crowding and environment (concentration, pH, and temperature) is evaluated using SANS and SAXS.

Rec1-resilin in uncrowded solutions→ radius of gyration Rg ~ 5 nm, and a scattering function for the triaxial ellipsoidal model best fit model.

On crowding (increase in concentration >10 wt %), Rec1-resilin molecules exert intermolecular repulsive force of interaction, the Rg value reduces with a progressive increase in concentration.

The structural organization of Rec1-resilin dynamically transforms from a rod (pH 2) to coil (pH 4.8) and to globular (pH 12) as a function of pH.

The temperature-triggered dual-phase-transition: rod-shaped below the upper critical solution temperature (~4 °C) and a large but compact structure above the lower critical solution temperature (~75 °C).



*Balu, R., Mata, J. P., Knott, R., Elvin, C. M., Hill, A. J., Choudhury, N. R., Dutta, N. K. (2016) *J. Phys. Chem. B* **120**, 6490-6503.

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Take Home Messages

- SANS is a powerful tool to study the global structures of isotropic systems in length scales ranging from 1 to 500 nm.
- Isotope replacement could enhance/vary the contrast without changing the chemistry of the systems.
- The scattering function is proportional to the product of contrast factor, form factor (intraparticle scattering function) and structure factor (interparticle interaction).
- Structural parameters can be obtained through model dependent approaches, while model independent scaling law can also reveal possible morphology of the studied system.
- Proposal deadline 15th September 2016 (for January 2017 to June 2017)

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