Small Angle X-ray Scattering

The last resort of the desperate!

Nick Terrill - Principal Beamline Scientist, Scattering, Diamond

SAXS at Diamond Beamline Progress and Science highlights

Small-angle, non-crystalline diffraction provides essential information on the structure and dynamics of large molecular assemblies in low ordered environments. These are characteristic of living organisms and many complex materials such as polymers and colloids.



SAXS at Diamond Beamline Progress and Science highlights

- Used for
 - Archaeology
 - Biology
 - Biomaterials
 - Ceramics
 - Colloids
 - Cultural heritage
 - Environmental science
 - Forensic science
 - Liquid crystals
 - Mineralised tissue
 - Polymers
 - Surfactants



Probing the Length Scales



Scattering

X-ray scattering is probing distances that are large compared to inter-atomic distances. Characteristics are:

Random orientation of particles (i.e. no long-range order) leads to scattering rather than diffraction (determination of size and shape)

Electron density variations at the particle-matrix interface cause x-rays to scatter.

The scattered intensity, I(q), is measured in terms of the scattering vector, q.

Scattering by two point centres



From G. Porod, Ch2 in "Glatter and Kratky"



X-ray scattering

Amplitude: $A(q) = \int_{Vr} \rho(r) e^{-ir \cdot q} dVr$ (Volume Integral)

Where $\rho(r)$ is the relates to the electron density and q is the scattering angle

Particle in solution => thermal motion => Particles have a random orientation/x-ray beam. The sample is **isotropic**. Only the **spherical average** of the scattered intensity is experimentally accessible.

Intensity:

 $I(q) = \langle A(q).A^*(q) \rangle$



Porod's law: specific surface and interface

 When two media are separated by a sharp interface, the scattered intensity follows an asymptotic law in the high q region:

$I(q)=Aq^{-4}+B.$

- This law is called the Porod's limit and has more sophisticated expressions in the case of complicated interfaces.
- The asymptotic value, when the electronic contrast of the sample is known, and when the intensity is expressed in absolute scale, allows the calculation of the specific surface S (in cm²/cm³) of the particles.



Surface Fractal Laws

• For a smooth surface $S(r) = r^2$, and for a rough surface $S(r) = r^{ds}$, where ds is the surface fractal dimension that varies from 2 to 3

-I(q) proportional to q^{ds-6}

 Surface fractals display power-law decays weaker than Porod's Law and are termed positive deviations from Porod's Law.





What do we mean by "size"?

Radius of gyration:

R_g² is the average squared distance of the scatterers from the centre of the object



 $R_g^2 = (1^2 + 1^2 + 1^2 + 2^2 + 2^2 + 3^2)/6 = 20/6$ $R_g^2 = \sqrt{3.333} = 1.82$



Form Factor for simple shapes



For more complicated shapes see reviews by J. S. Pedersen – http://www.chem.au.dk/~jansp/resdescription.html



Solution SAXS: R_g , I_0 and P(r)





SAXS studies on silica templated with polyelectrolyte-surfactant complexes





Bin Yang, Robben Jaber, and Karen J. Edler, Langmuir, 2012, 28 (22), 8337, DOI: 10.1021/la3014317







1.0

20

r (Å)

p(r) 0.5

UNIVERSITY OF







Melanie C. O'Sullivan, Johannes K. Sprafke, Dmitry Kondratuk, Corentin Rinfray, Timothy D. W. Claridge, Alex Saywell, Matthew O. Blunt, James N. O'Shea, Peter H. Beton, Marc Malfois, Harry L. Anderson, Nature Letters Volume: 469, Pages: 72–75, 2011

10 20

50 60 70

r (Â)

30 40

Size polydispersity

$$I(q) = \Delta \rho^{2} \int_{0}^{\infty} P(q, R) D(R, \sigma_{R}) dR$$

$$P(q, R) = \left[V \frac{3[\sin(qR) - qR\cos(qR)]}{(qR)^{3}} \right]^{2}$$

$$D(R, \sigma_{R}) = \frac{1}{\sigma_{R} \sqrt{2\pi}} \exp\left[-\frac{(R - R_{a})^{2}}{2\sigma_{R}^{2}} \right]$$

$$P(q, R) = \frac{1}{\sigma_{R} \sqrt{2\pi}} \exp\left[-\frac{(R - R_{a})^{2}}{2\sigma_{R}^{2}} \right]$$

100

Size polydispersity

Smeared form factor P(q) for a sphere vs q showing the damping of Porod oscillation with increasing polydispersity (σ_{eff}). The oscillations disappear for $\sigma_{eff} > \sim 0.21$. The mean particle diameter $a_0 = 100$ nm for all calculations. Note the overall q⁻⁴ power law for q >0.01nm⁻¹. The calculations terminate in the Guinier regime at low q.

Gold colloid

The spherical gold colloidal

R_{av} = 25.5 Å

σ = 4.4 Å

D (nm)

(x 10⁻¹³

18.6

1.2

18.0

2.3

55.0

0.5

28.0

0.5

39.1

1.0

26.8

1.3

19.8

0.6

18.8

1.6

The Stability of Silver Nanoparticles in a Model of Pulmonary Surfactant

pH 3 (with DPPC)

Irreversible

coarsening

Agglomeration

Charge screening

Loss of Citrate Cap

Bey Fen Leo, Shu Chen, Yoshihiko Kyo, Karla-Luise Herpoldt, Nicholas J. Terrill, Iain E. Dunlop, David S. McPhail, Milo S. Shaffer, Stephan Schwander, Andrew Gow, Junfeng Zhang, Kian Fan Chung, Teresa D. Tetley, Alexandra E. Porter, and Mary P. Ryan, Environ. Sci. Technol. 2013, 47, 11232–11240, DOI: 10.1021/es403377p front of the Huns local

Charge stabilised NPs

Iron oxyhydroxides in the environment

Thermodynamics vs. Kinetics

- Most stable phases are goethite (FeOOH) and hematite (Fe₂O₃)
- Poorly-ordered iron oxyhydroxide (ferrihydrite) very common in soils and sediments

Schwertmannite $Fe_{16}O_{16}(OH)_{12}(SO_4)_2$

Ferrihydrite Fe_xO_yOH_z.nH₃O

(Janney et al., 2000)

Shaw et al

Pair/Size distribution function (pure) (PDF/SDF)

Pair distribution function

(Rg more accurate: based on full scattering pattern not only low q)

- Equant particle shape at beginning of reaction
- Elongated particles forming by end of reaction

Size distribution function

(degree of polydispersity)

- Monodispersed system at beginning of reaction
- Slight increase in polydispersity with time

pH = 4

ASAXS example from BESSY (Berlin)

What if you have a Non-Dilute system?

- Scattering (Interference) determined by spatial dimensions
- Form Factor P(q) particle size and shape (intraparticle)
- Structure Factor S(q) interparticle correlations function of local order and interaction potential; complex if correlation between position and orientation

Concentration effects (S_q)

Figure 1: Cross-section for several different volume fractions of PS spheres in glycerol vs. QR.

Small Angle X-ray Scattering Study of a Hard-Sphere Suspension: Concentrated Polystyrene Latex Spheres in Glycerol

L. B. Lurio¹, D. Lumma¹, A. R. Sandy¹, M. A. Borthwick¹, P. Falus¹, S. G. J. Mochrie¹, J. F. Pelletier², M. Sutton², Lynne Regan³, A. Malik⁴ and G. B. Stephenson⁴

Semicrystalline Block Copolymers

- Few commercial examples
- Crystallisable end blocks
- PE-PEP-PE (hPB-hPI-hPB)
- Low crystallinity PE look-alike
- Metallocenes for multi-blocks
- Very complicated phenomenology Break-out & confined crystallisation depending on morphology and T_a of noncrystallising material.

Spherulite $O(10 \ \mu m)$

Lamella O(10-100 nm)

diamond

Bragg's law gives an estimate of interference function $d=2\pi/q^*$ but how do we get the degree crystallinity and hence L?

The scattering invariant $Q = \phi(1-\phi)\Delta n^2$ $Q = \int I(q)q^2 dq$ with limits $0 \le q \le \infty$ But the SAXS pattern has data in a range of q

Scattering at Small Angle

semicrystalline lamellar stacks

η

SAXS Invariant

1.2

 $Q = \phi(1-\phi)\Delta\eta^2$ ϕ and $\Delta\eta$ in a lamellar stack do not change during crystallisation but the crystalline volume increases so

 $Q = X_s$ the volume fraction of spherulites Kinetics from time-resolved (static) scattering

WAXS

degree of crystallinity $X_c = A_c/(A_c + A_a)$

How does it work?

Added Value from the sample

Block Copolymer Self Assembly

At high T thermal motion overcomes unfavourable interactions between blue and red segments

increasing B fraction

free energy = separation - stretching - interfacial energy

Lamellar phase

diamond S. Förster

 $Peak order - q_0, 2q_0, 3q_0, 4q_0$

Hexagonal phase

diamond S. Förster

Body Centred Cubic

la3d Gyroid

Khandpur et al Macromolecules 1995

A real time SAXS study of oriented block copolymers during fast cyclical deformation, with potential application for prosthetic heart valves

- Study of a range of thermoplastic elastomers with all rubbery components in the block copolymers
 - Time resolution of RAPID 10ms used (although trials of <1ms also proved successful)
- Cycling used to mimic conditions for a prosthetic heat valve (10,000 cycles)

Time resolved X-ray diffraction studies of drug induced membrane degradation

0.005

0.010

0.015

S/ Å'

0.020

0.025

Automated high pressure cell for pressure jump x-ray diffraction, Nick Brooks, Beatrice Gauthe, Nicholas Terrill, Sarah Rogers, Richard Templer, Oscar Ces, John Seddon (2010) *Review of Scientific Instruments* 81:064103 DOI: 10.1063/1.3449332

University of BRISTOL Electric Field Induced Orientational Order in Suspensions of Anisotropic

Nanoparticles 2D Detector

Scattering pattern obtained from Permanent Rubine in dodecane (30 wt%) using short camera length with (a) zero field (b) Electric field applied (4V=mm) giving nematic

phase.

Robert Greasty, Jana Heuer, Susanne Klein, Claire Pizzey, and Robert Richardson Mol. Cryst. Liq. Cryst., 545, 133

Microfocus End Station

Queen Mary Nanoscale Fracture Mechanisms in Fibrolamellar Bone in Bending and Compression

FWHMy: 10.8 µm

FWHM_H: 11.7 µm

Microfocus spot obtained on I22 with CRL (90 lenses) at 14 keV

Angelo Karunaratne, Christopher R Esapa, Jennifer Hiller, Alan Boyde, Rosie Head, JH Duncan Bassett, Nicholas J Terrill, Graham R Williams, Matthew A Brown, Peter I Croucher, Steve DM Brown, Roger D Cox, Asa H Barber, Rajesh V Thakker, and Himadri S Gupta, Journal of Bone and Mineral Research, Vol. 27, 2012, 876.

Tablet Compaction and its effect on pharmaceutical activity

Tablet Test shapes including representative indentation types

Compaction/ Morphology

Orientation around compaction site

Relative density 0.94 0.93 0.92 0.91 0.90 0.89 0.88 0.87 0.86 0.85 0.84 0.83 0.82

Data Collection via GDA

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Data Reduction

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Detector Corrections 1D/2D

HOL Fropogation

Background Subtractions 1D/2D

Absolute intensity 1D/2D

Radial Averaging

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Dark Current, Detector Response, etc.

Sample cell, Porod, amorphous (variable) in wis Proposation

diamond

By Cross calibration or directly

Sector and full circle with masking

Data Calibration & Reduction in Dawn

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Data Analysis

- Peaks and single parameter values are being integrated into DAWN.
- More detailed analysis is available via a range of packages that have been developed to focus on particular areas of science or experiment.

I22 – Small Angle X-ray Scattering for Diamond

Beamline:

Energy Range 3.7-20keV d/Å range 1-5000Å (probably >1mm)

Beam size:

 $70\mu m (V) - 330\mu m(H)$ $6\mu m \times 7\mu m$ with microfocusing

End Station:

Flexible Sample platform Inline sample viewing (Microfocus)

Small Angle Scattering (SAXS)

- O. Glatter and O. Kratky "Small Angle X-Ray Scattering" (http://physchem.kfunigraz.ac.at/sm/Software.htm)
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Thanks for your attention

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