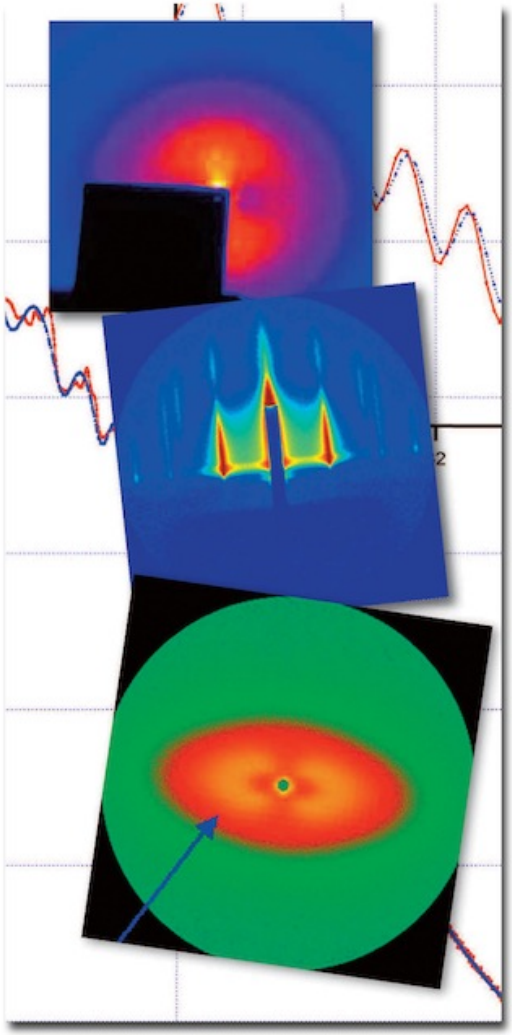
Small-Angle Scattering: Theory and Applications



Small-Angle Scattering Short Course 2013: ***Beyond R_G***

Advanced Photon Source

Argonne National Laboratory. Argonne, IL USA

2013-10-28

Pete R. Jemian

Contributions: Jan Ilavsky, Dale Schaefer, Ulla Vainio

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Syllabus: Small-Angle Scattering Theory

- Why small-angle scattering?
- Basic SAS Theory
  - Scattering length density and Babinet's Principle
  - Radius of gyration
  - Approximations: Invariant, Guinier, and Porod
  - Form Factor
- SAS Theory Beyond R_G
  - Scattering Interference
  - Particle size distributions
  - Contrast variation
  - Fractals
  - Grazing incidence
- Applications will appear throughout

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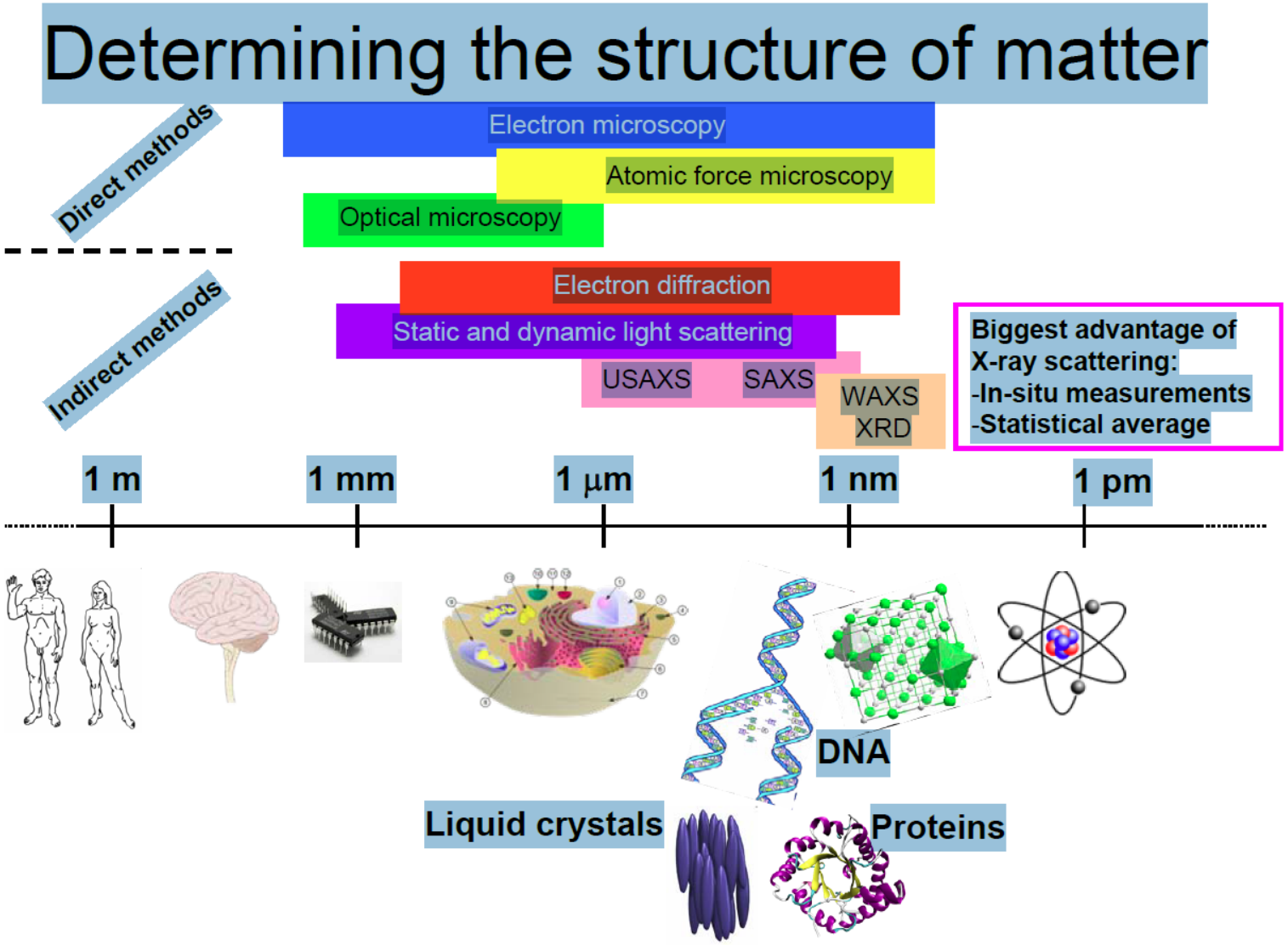
Why Small-Angle Scattering?

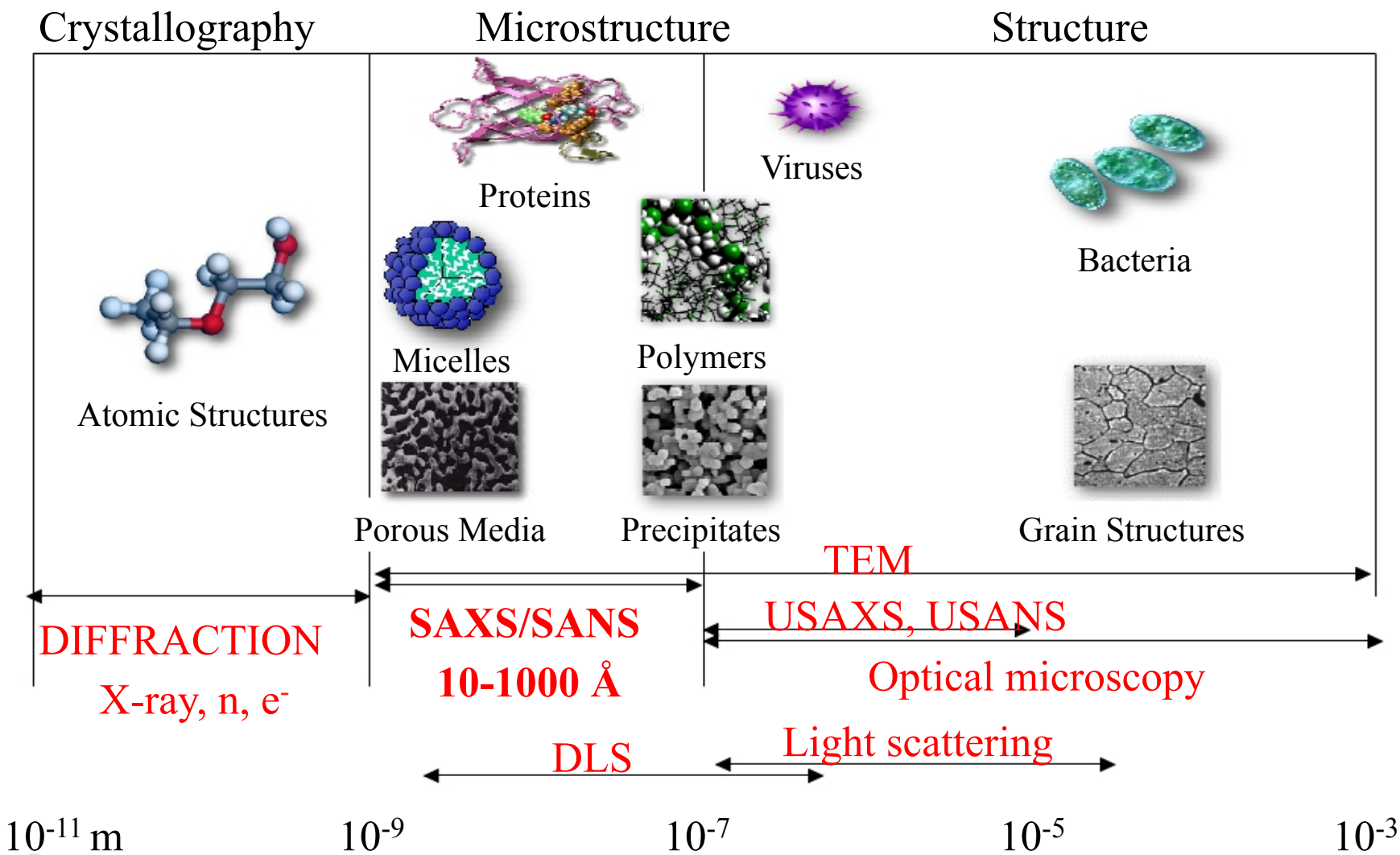
- Premier **method for size characterization of** nanoscale density **inhomogeneities**
- Results are statistically significant
- Studies complement other methods
- Applicable to wide variety of technologically important materials
- Indirect measure of size, amount, or shape
- Easy experiment, harder analysis
- Sample in transmission, $t=1/\mu$
- Monochromatic radiation ($\Delta\lambda/\lambda$ up to 25% is acceptable)
- X-ray or neutron radiation sources can probe optically opaque substances

Length scales of characterization techniques



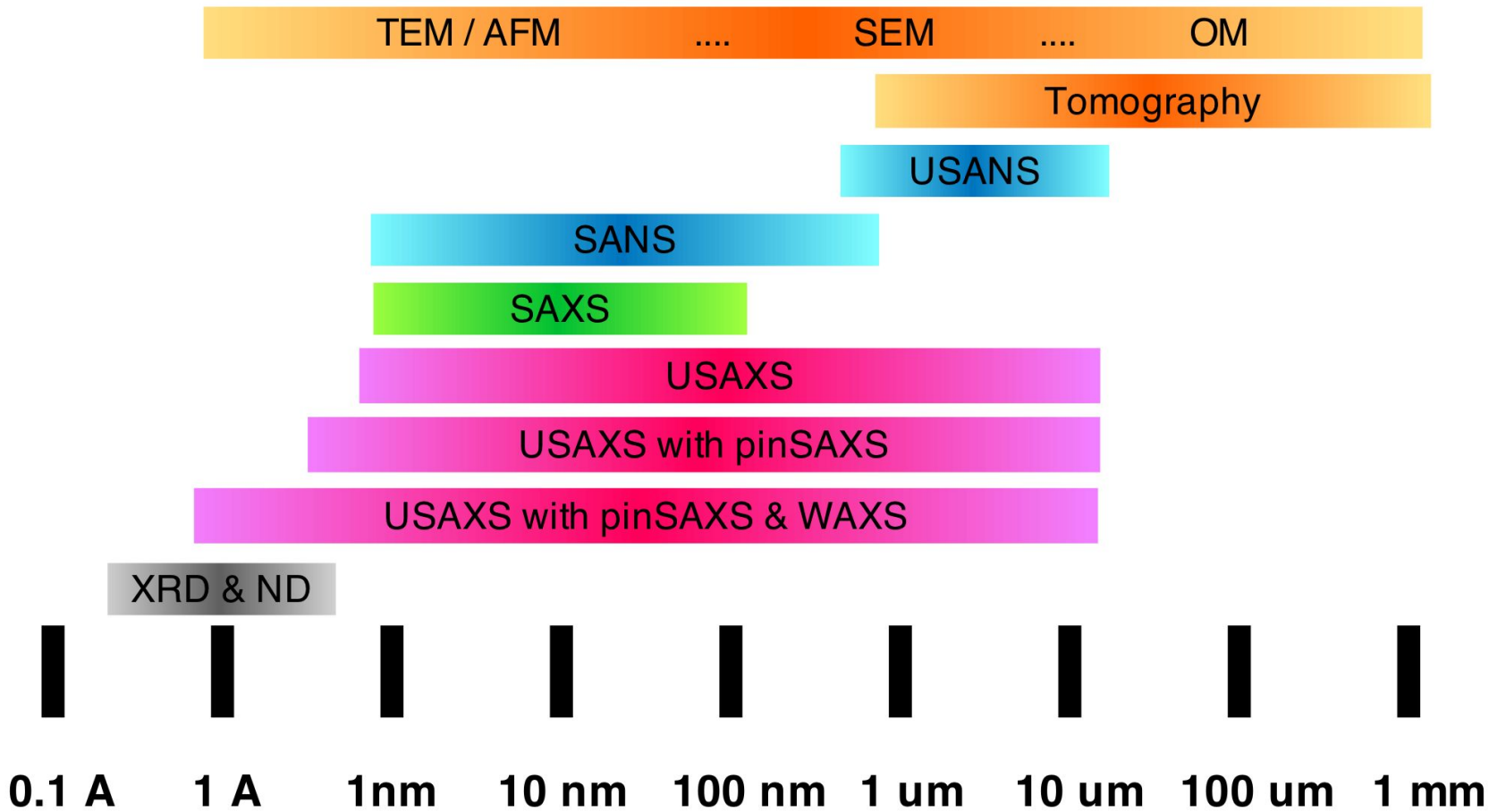
source: U. Vainio; 2010 DESY summer school lectures

Length scales probed by SAS and other characterization techniques



Source: Jan Ilavsky, private communications

Length scales: SAS and other techniques



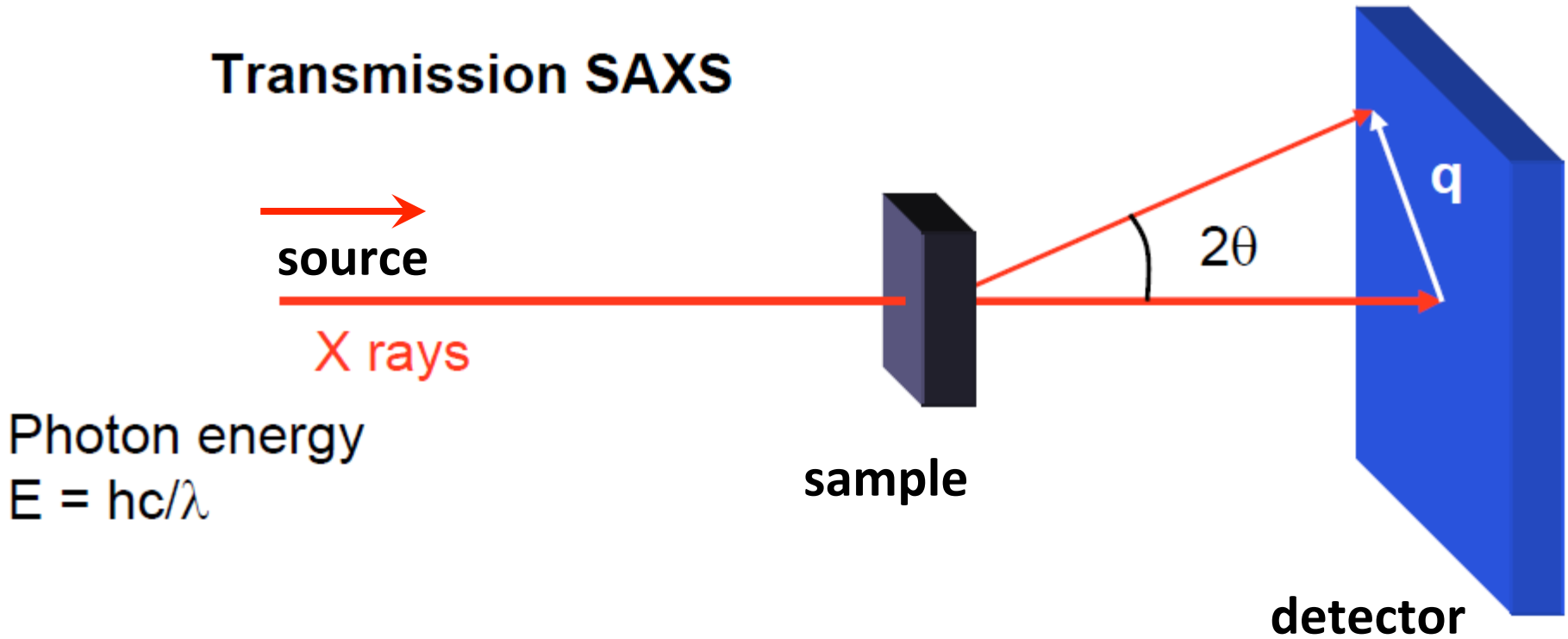
Source: Jan Ilavsky, private communications

What types of materials can be investigated with Small-Angle Scattering?

- Not limited to just these …
- Materials science:
  - PS spheres: diameter & polydispersity
  - Depletion restabilization of colloidal silica
  - Microstructure of porous silica precursor bodies
  - Yttria-stabilized zirconia
  - Paint pigment
  - Colloidal silica
- Human medicine
  - Toughening of PMMA bone cement
- Environmental science
  - Yucca Mountain Groundwater Colloids
- Anomalous scattering contrast variation
  - Silicon Nitride for gas turbine engines
  - Stability of modified Fe9Cr1Mo Steel at high service temperatures

- Samples with nanoscale density inhomogeneities
- Samples that can transmit > few percent of beam

SAS in Transmission with area detection



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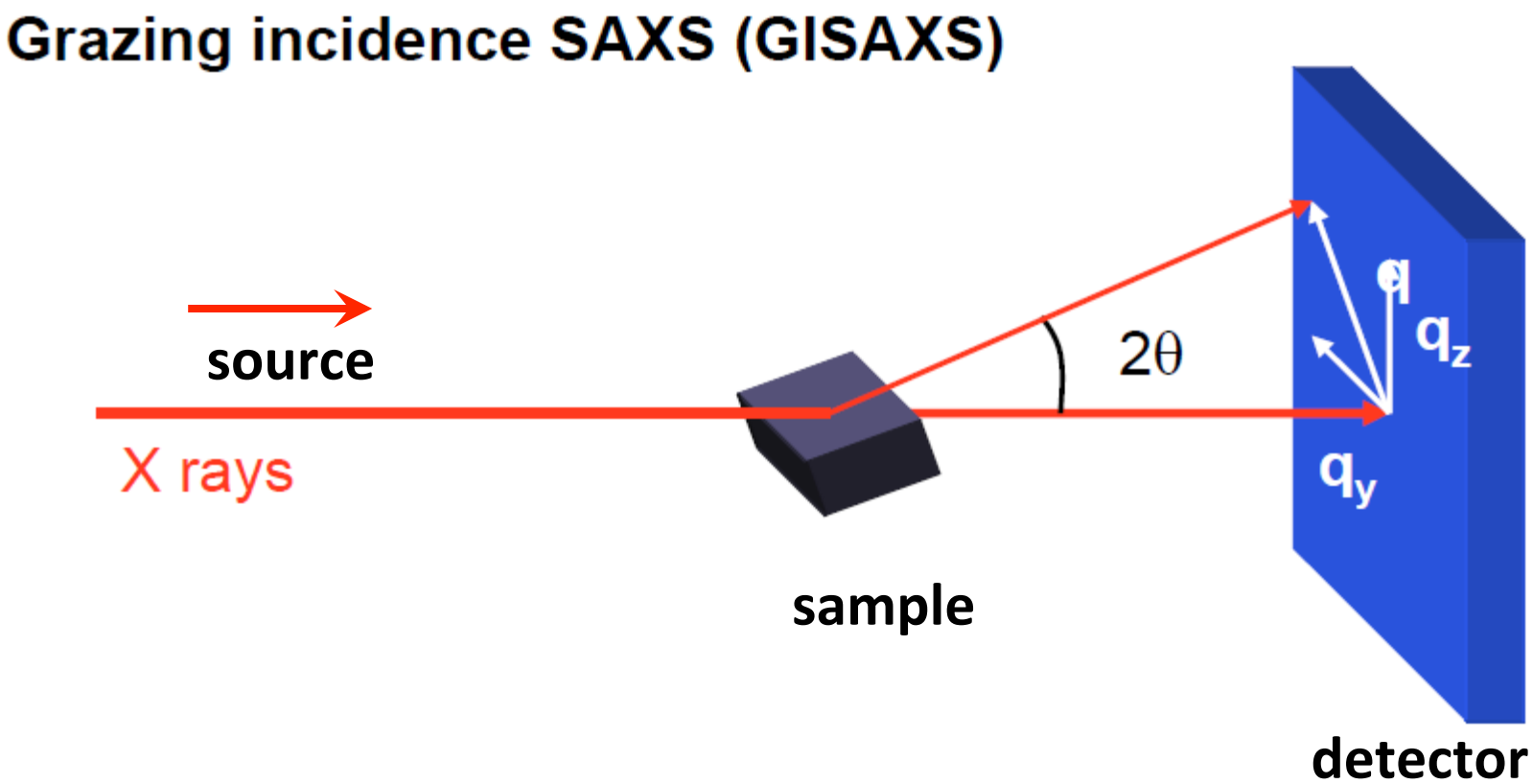
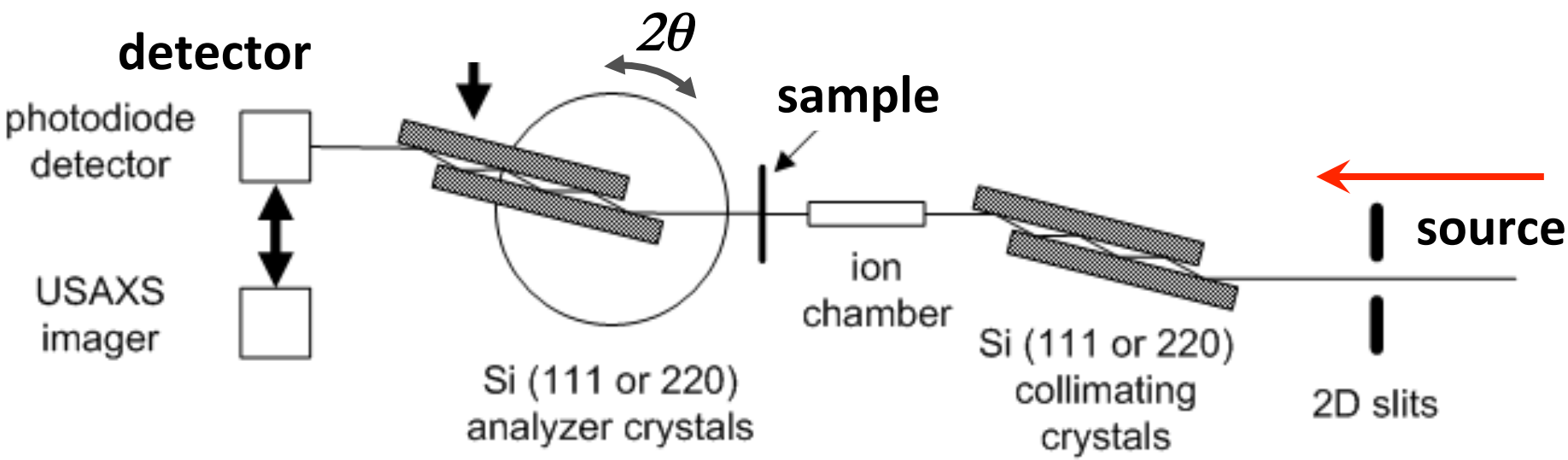
SAS in Grazing Incidence



source: U. Vainio; 2010 DESY summer school lectures

SAS in transmission with Bonse-Hart camera

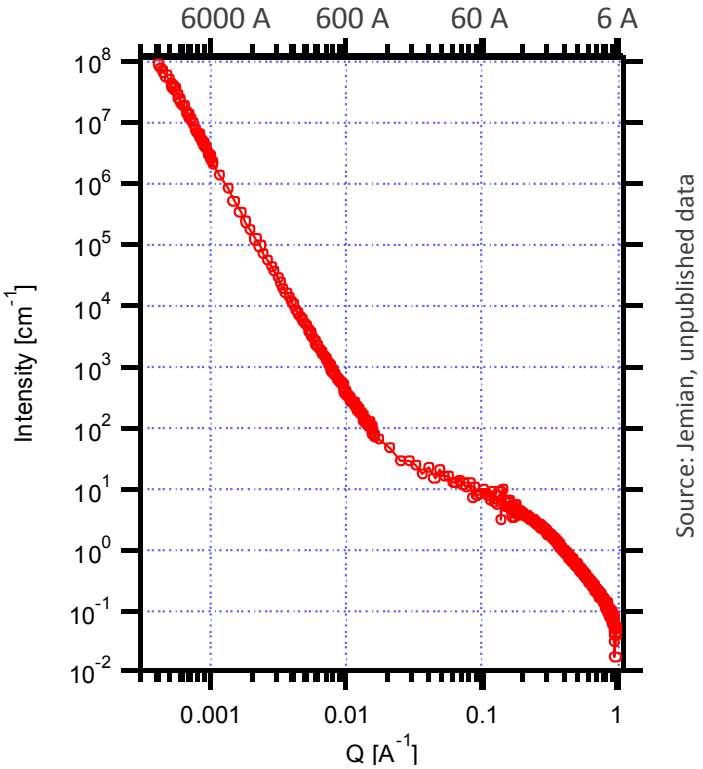


J Appl Cryst 42.3 (2009) 469-479
Metall Mater Trans A 44.1 (2013) 68-76
http://usaxs.xray.aps.anl.gov/docs/overview/publications.html

What can be learned from a Small-Angle Scattering Experiment?

- Size of scatterer
- Amount of scatterers
- Polydispersity
- Distribution of scatterers
- Shape of scatterers
- Morphology of scatterers
- Composition of scatterers

* *scatterer*: density inhomogeneity strongest contribution at $Q = 2\pi/l$



- There is *strong* dependence between some of these terms.
- SAS experiments, *complemented by other measurements*, can yield rich information about the microstructure.

Need for complementary methods

The richness of an integrated approach to materials characterization is dependent on the availability of complementary methods.

The more you know
the more you can learn.

Example: M_2C in AF1410 Steel

Complementary Methods:
XRD, TEM, AP/FIM, SANS,
mechanical properties,
thermodynamics calculations

SANS results bridged gap between TEM & AP/FIM size data
Also provided new information of volume fraction and number density

J.S. Montgomery, 1990,
Ph. D. Thesis, Northwestern University.

A.J. Allen, D. Gavillet, and J.R. Weertman;
***Acta Metall* 41** (1993) 1869-1884.

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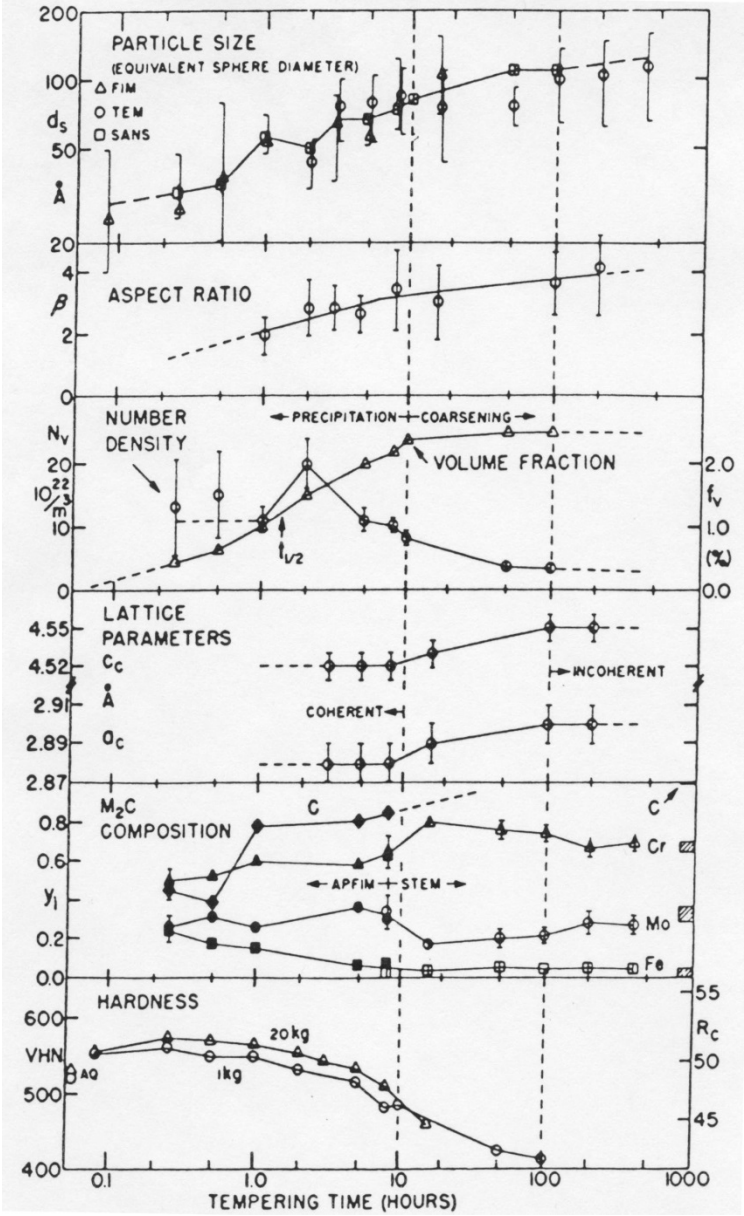

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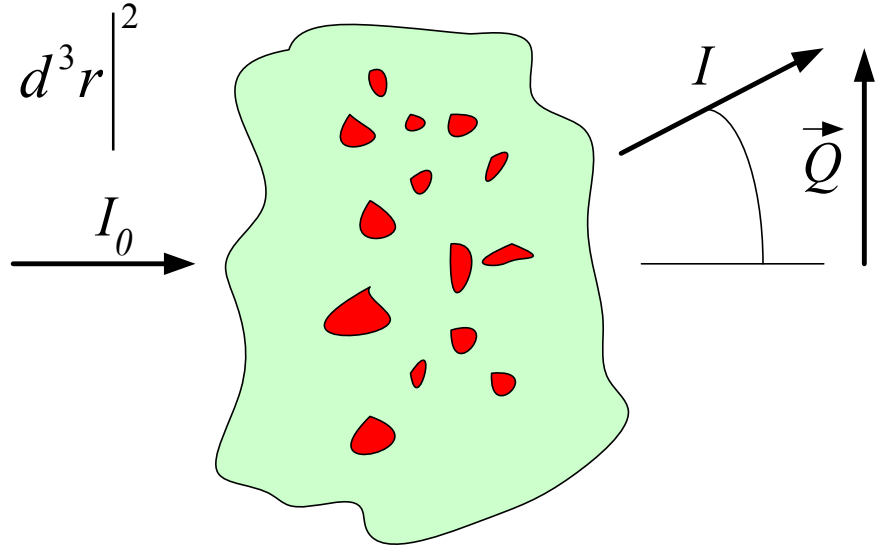
Origin of scattering

- Scattering is due to inhomogeneities in scattering length density, ρ
- Scatterers are homogeneous
- Surroundings are homogeneous
- Radiation is scattered only once or not at all (no multiple scattering)

$$I(Q) \propto \frac{d\Sigma}{d\Omega}(Q) = \left| V_p^{-1} \int_{V_p^{-1}} \rho(r)\, e^{-Q\cdot r}\, d^3 r \right|^2$$

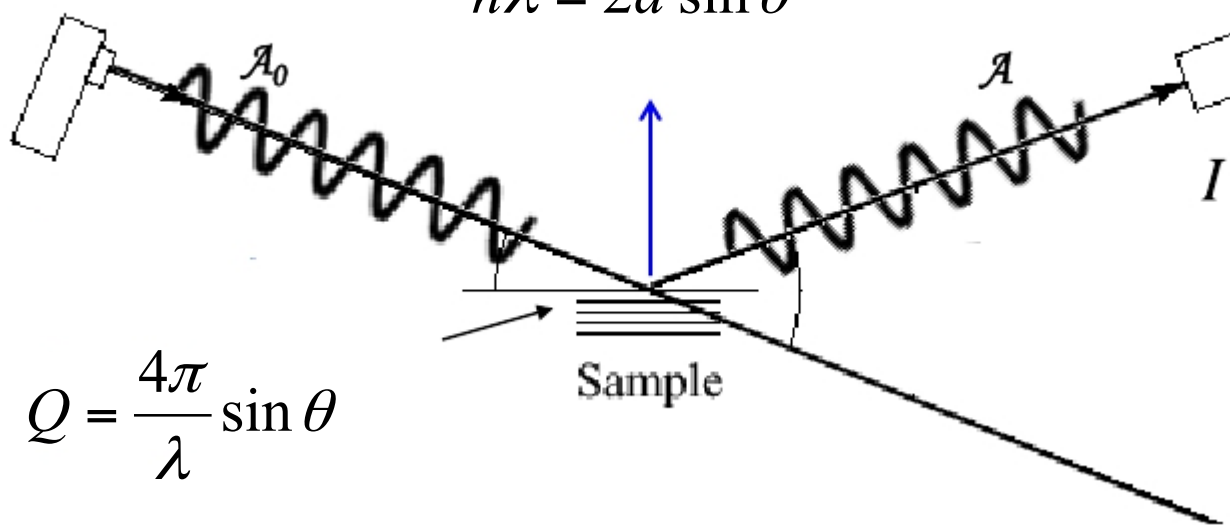


$$Q = \frac{4\pi}{\lambda} \sin\theta$$

Crystals: Bragg's Law and the scattering vector *Q*

$$n\lambda = 2d\sin\theta$$

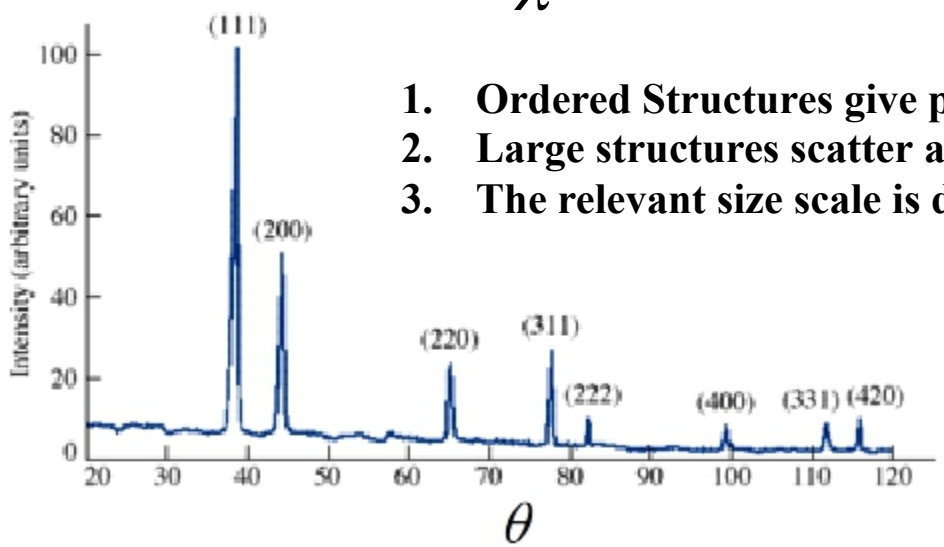
$$d = \frac{2\pi}{Q}$$



$$I = \left(\frac{\mathcal{A}}{\mathcal{A}_0}\right)^2$$

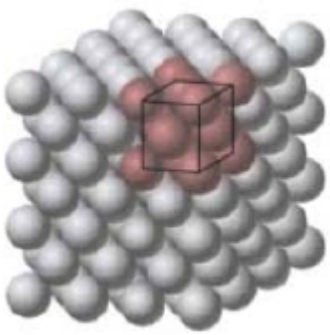
$$Q = \frac{4\pi}{\lambda}\sin\theta$$

Reciprocal space



1. **Ordered Structures give peaks in "reciprocal" Space.**
2. **Large structures scatter at small angles.**
3. **The relevant size scale is determined by $2\pi/q$**

real space



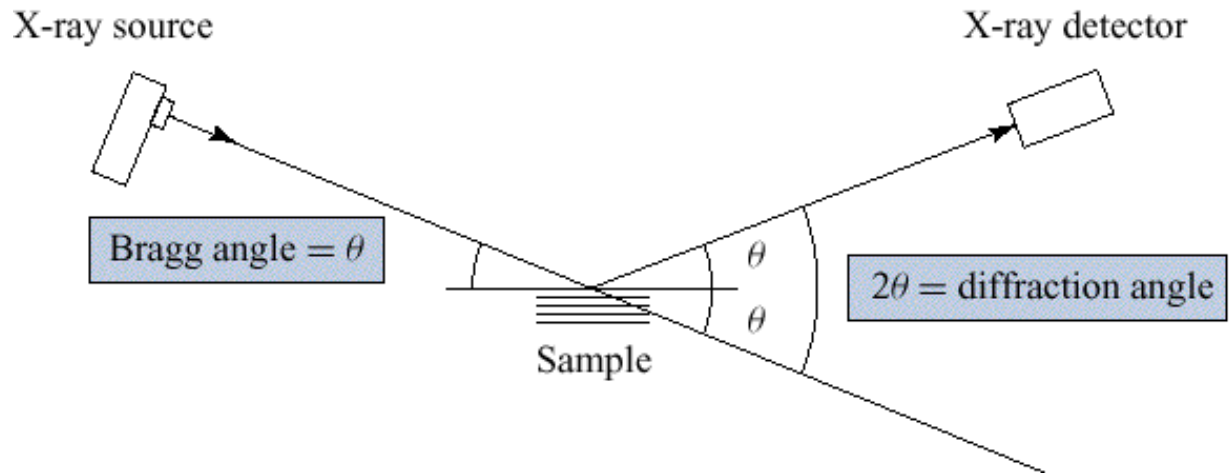
Problem: Nano-to-micromaterials are seldom ordered

Dale Schaefer, private communications

Sizes measured

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

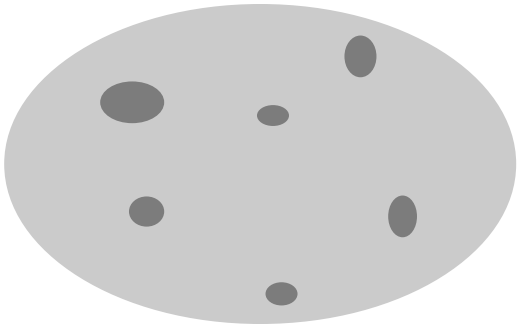
$$d = \frac{2\pi}{Q}$$



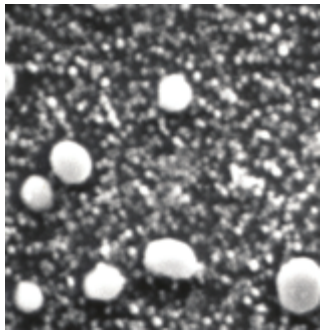
Q [A^{-1}]	D [nm]	2Θ [deg] 12keV
1	0.6	10
0.1	6	1
0.01	60	0.1
0.001	600	0.01
0.0002	3000 (3 um)	0.001

Detector dynamic range is important – Intensity ~ q^{-4}

Scattering length density



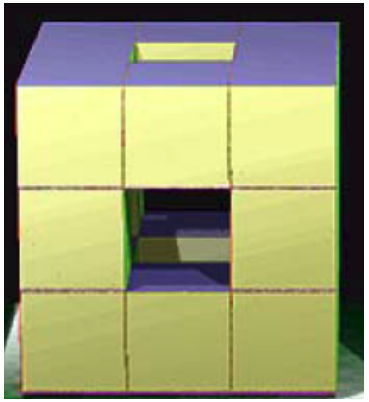
- Measure of interaction difference of radiation with atoms/molecules in scatterer (density inhomogeneity) and its surroundings
- Scattering is due to a difference in:
  - X-ray: refractive index, $r_{e-}f$
  - neutron: nuclear (and magnetic) scattering length



Precipitation in commercial Waspaloy

$$\rho_{sld} = \frac{n}{V} b \qquad \Delta\rho = r_{e-} \sum_Z \Delta c_Z f_Z$$

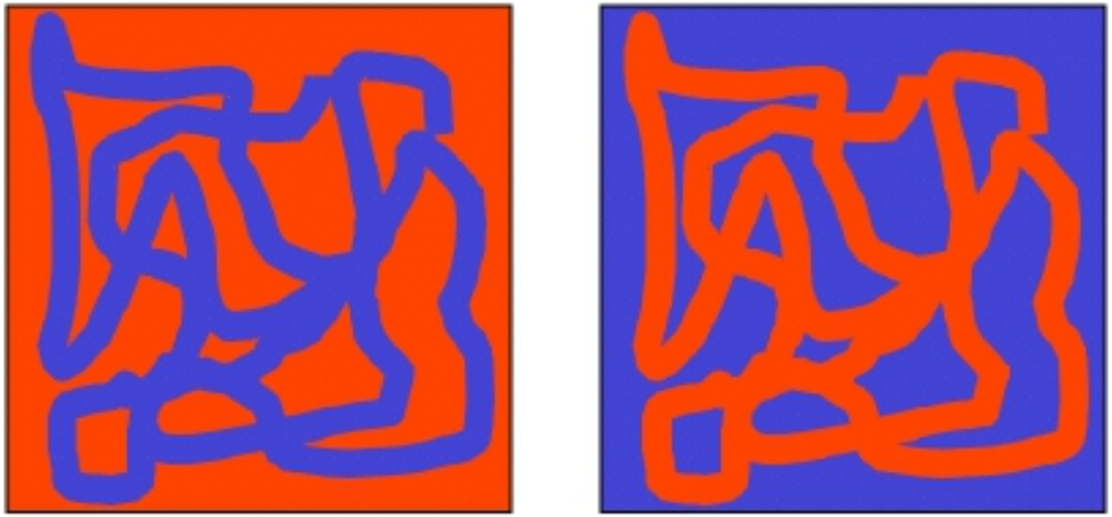
- n: number of atoms/molecules
- V: unit volume
- b: scattering length
- r_{e-} : Thompson radius of an electron, 2.818 fm
- f: atomic scattering factor



Source: http://commons.wikimedia.org/wiki/File:Menger_sponge_(Level_1-4).jpg

Babinet's Principle

- Two structures give the same scattering (*)
- Contrast is relative
- Loss of phase information
- Very important in multi-phase systems for contrast matching or variation



$$\frac{d\Sigma}{d\Omega}(\vec{\mathbf{q}}) \propto (\rho_1 - \rho_2)^2$$

*incoherent scattering may be different

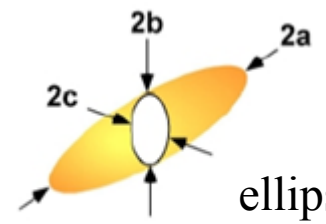
Radius of gyration, R_g

- Radius of gyration, R_g, is the name of several related measures of the size of an object, a surface, or an ensemble of points *of any geometry*. It is calculated as the root mean square distance of the object's parts from its center of gravity.
- In polymer physics, the radius of gyration is proportional to the root mean square distance between the parts of the object:

$$R_g^2 = \frac{\int r^2 \rho(r) dr}{\int \rho(r) dr}$$

Gaussian chain

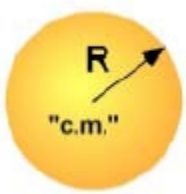
$$\langle R_g^2 \rangle = N \frac{l^2}{6}$$



ellipsoid

$$R_g^2 = \frac{1}{5}(a^2 + b^2 + c^2)$$

Sphere



$$R_g^2 = \frac{3}{5} R^2$$

Thin rod

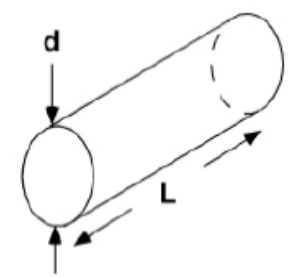
$$R_g{}^2 = \frac{L^2}{12}$$

Thin disc

$$R_g{}^2 = \frac{R^2}{2}$$

Cylinder

$$R_g{}^2 = \frac{R^2}{2} + \frac{L^2}{12}$$



Basic measures from a Small-Angle Scattering experiment

Guinier law $$\lim_{Q\to 0} I(Q) = I(0)\exp\left(-\frac{1}{3}R_G^2 Q^2\right)$$

$$Q_{\max} R_G < 1.2$$

Porod law $$\lim_{Q\to\infty} I(Q) = 2\pi\, S_V \left|\Delta\rho\right|^2 Q^{-4}$$

$$Q_{\min} D > 3$$

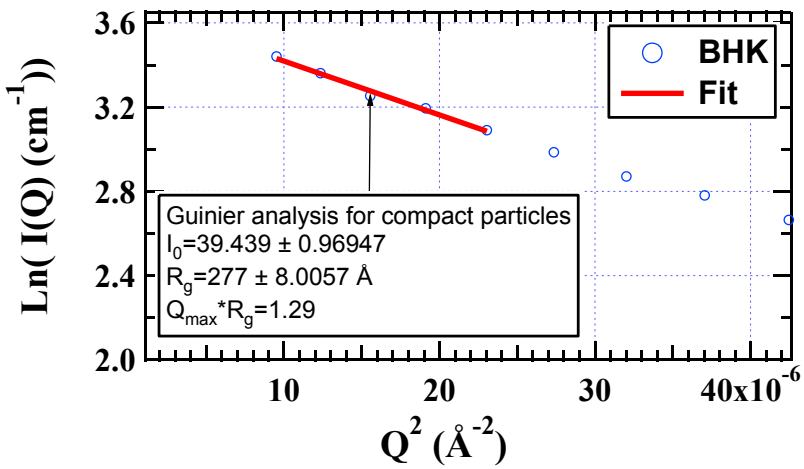
invariant $$2\pi^2 V_V \left(1 - V_V\right)\left|\Delta\rho\right|^2 = \int_0^\infty Q^2 I(Q)\, dQ$$

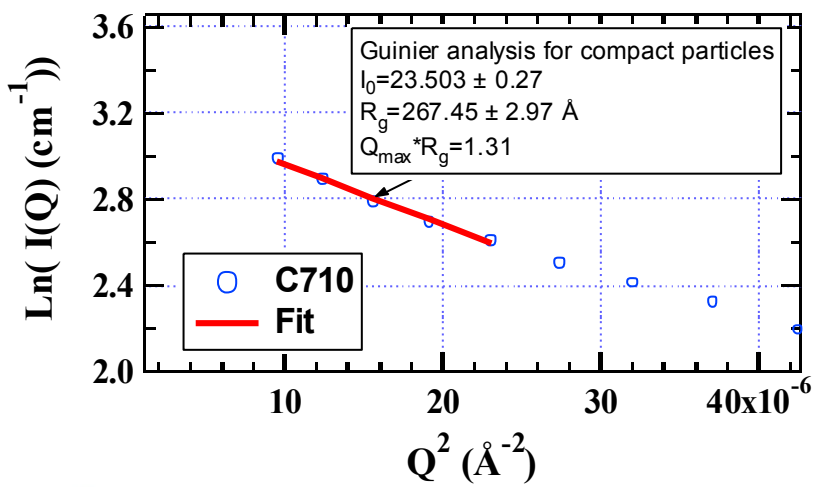
Hands-on Application

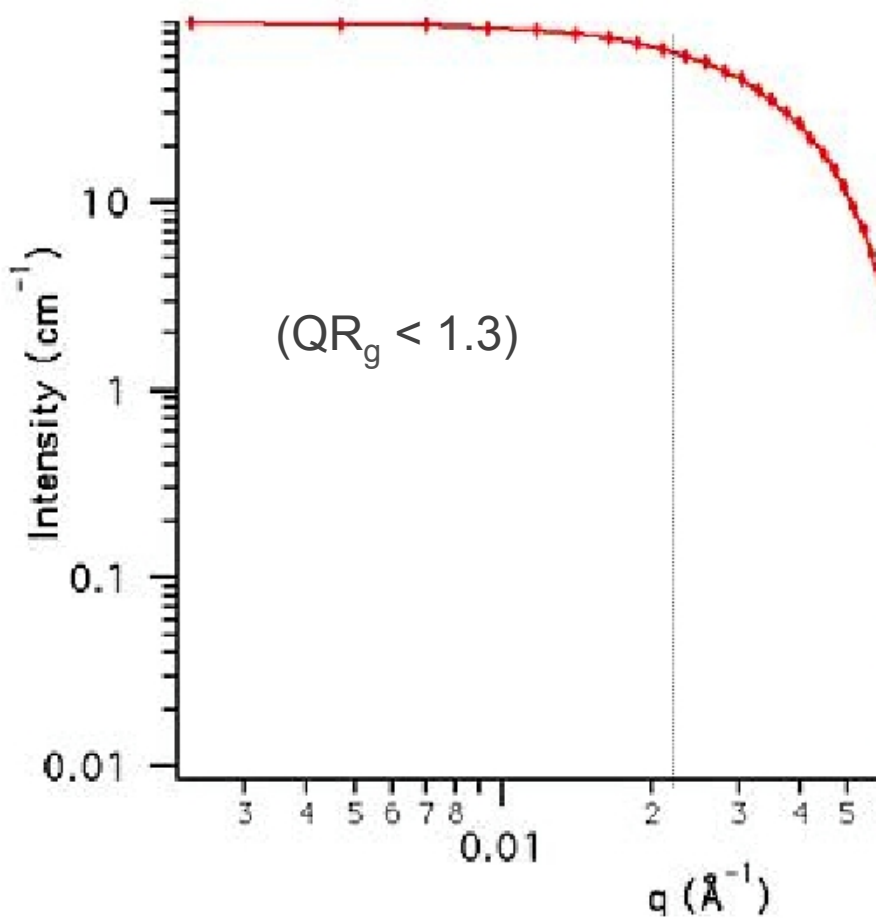
Let's apply our understanding to a few real examples

Example Fit to Guinier Approximation

$$I(q) \propto \exp(-Q^2 R_g^{\ 2} / 3)$$

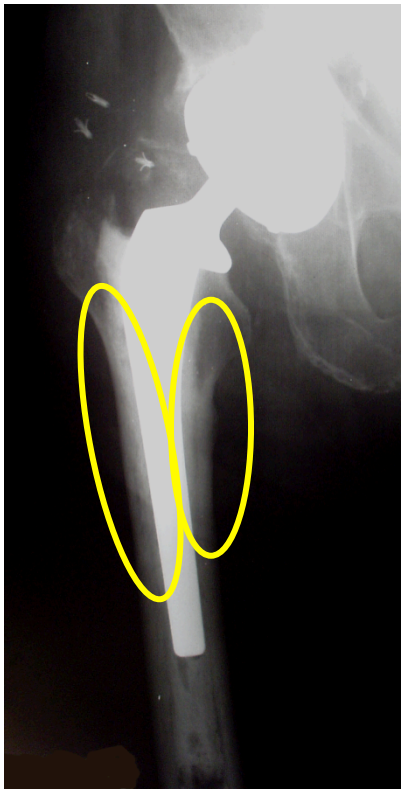






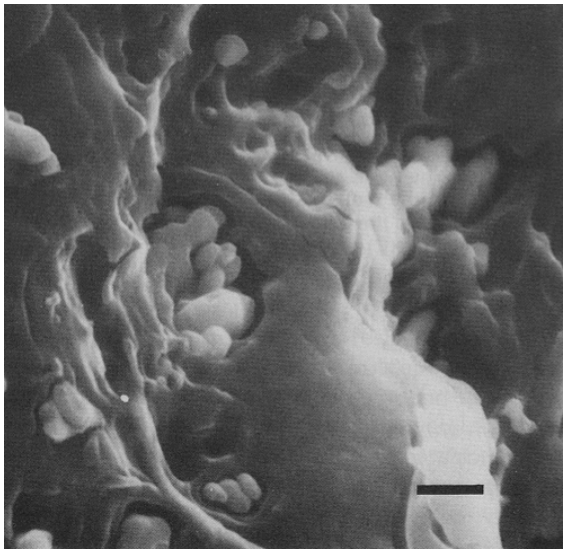
Source: Jan Ilavsky, private communications

Barium Sulfate added as radiopacifier to PMMA Bone Cement



Bellare, private communications

agglomeration

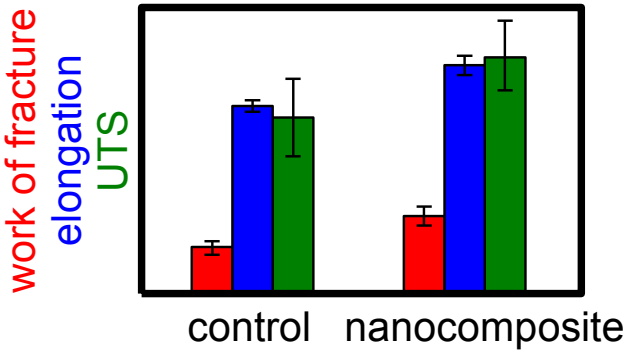


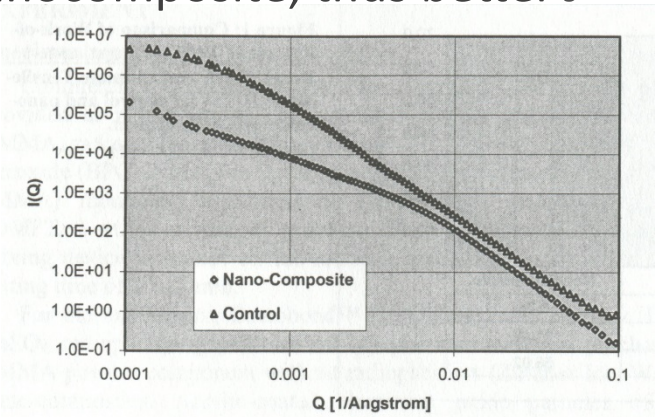
Topoleski et al, J. Biomed Mater. Res., 1990

Various Bone Cements	Impact Strength (J)
Simplex	0.333± 0.02
Palacos R	0.402± 0.03
Palacos K	0.382± 0.03
CMW – 0	**0.578**± 0.06
CMW+4% BaSO4	**0.323**± 0.03
CMW+8% BaSO4	**0.274**± 0.03
CMW+4.2% Erythocyne	0.461± 0.03
CMW+8% BaSO4+4.2%Ery	0.372± 0.03

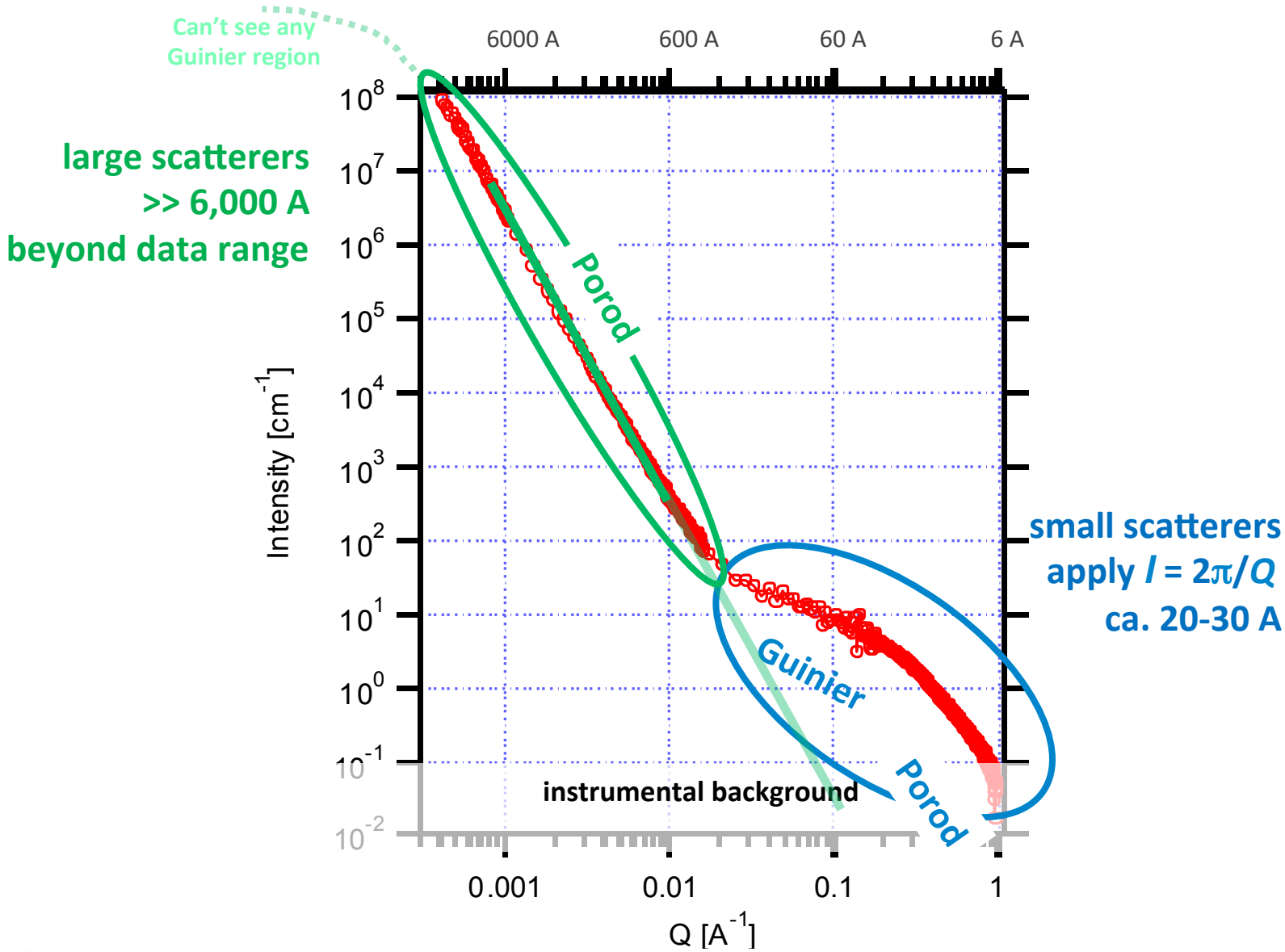
de Wijn et al, Acta Orthop Scand, 1975

No agglomeration with nanocomposite, thus better *J*





Let's look at that earlier figure



Intermission

Information Obtained from Quantitative Small-Angle Scattering

volume fraction

$$V_V = \sum_i f_i(D)\Delta D_i$$

number density

$$N_V = \sum_i \frac{f_i(D)\Delta D_i}{\left(\pi/6\right)D_i^3}$$

Radius of gyration

$$R_G = \sqrt{\langle r^8 \rangle / \langle r^6 \rangle}$$

specific surface

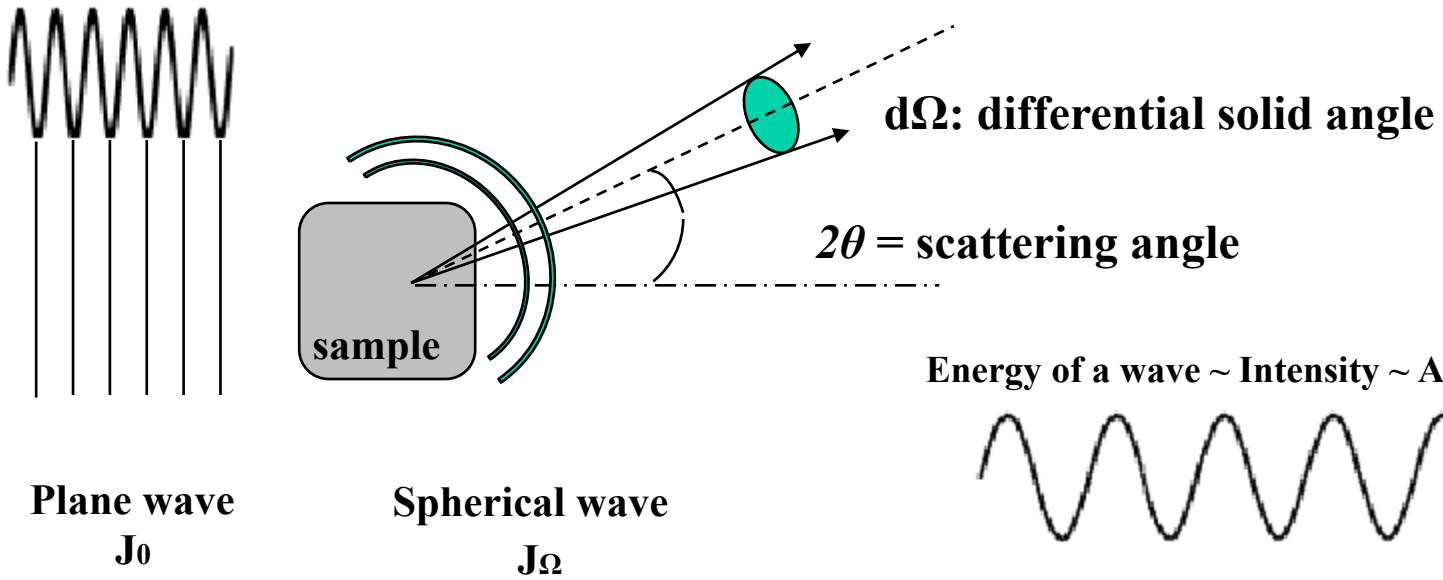
$$S_V = 6\sum_i f_i(D)\frac{\Delta D_i}{D_i}$$

mean spacing

$$\Lambda = \left(N_V\right)^{-1/3}$$

	volume-weighted	number-weighted
mean diameter	$\overline{D}_V = V_V^{-1}\left[\sum_i D_i f_i(D)\Delta D_i\right]$	$\overline{D}_N = N_V^{-1}\left[\sum_i D_i \frac{f_i(D)\Delta D_i}{\left(\pi/6\right)D_i^3}\right]$
standard deviation	$\sigma\left(\overline{D}_V\right) = \sqrt{V_V^{-1}\left[\sum_i D_i^2 f_i(D)\Delta D_i\right] - \left(\overline{D}_V\right)^2}$	$\sigma\left(\overline{D}_N\right) = \sqrt{N_V^{-1}\left[\sum_i D_i^2 \frac{f_i(D)\Delta D_i}{\left(\pi/6\right)D_i^3}\right] - \left(\overline{D}_N\right)^2}$

Intensity and Differential Scattering Cross Section



Energy of a wave ~ Intensity ~ Amplitude^2 = $|\mathcal{A}|^2$

Spherical wave:	**Flux J_Ω =**	**energy/unit solid angle/s** **or**	**photons/ unit solid angle /s**
Plane wave:	**Flux J_0 =**	**energy/unit area/s** **or**	**photons/unit area/s**

$$\frac{J_\Omega}{J_0} = \frac{d\sigma}{d\Omega}$$ differential scattering cross section *per atom* per unit solid angle

$$\frac{d\Sigma}{d\Omega} = \frac{1}{V}\frac{d\sigma}{d\Omega}$$ differential scattering cross section *per unit sample volume* per unit solid angle

Dale Schaefer, private communications

Form Factor of a sphere

$$\mathcal{A}_1(\boldsymbol{q}) = \frac{A(\boldsymbol{q})}{A_0} = \int \rho(\boldsymbol{r}) e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} d\mathbf{r}$$

$$= \int_0^\infty \rho(r) 4\pi r^2 \frac{\sin qr}{qr} dr$$

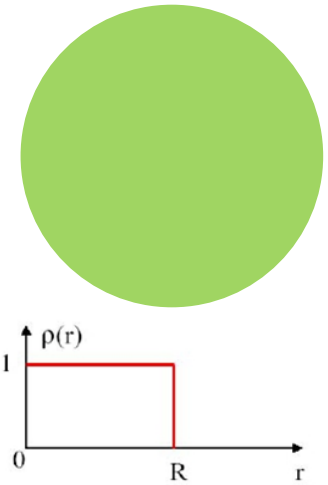
$$= \frac{\rho_0 4\pi}{q} \int_0^R r \sin(qr)\, dr$$

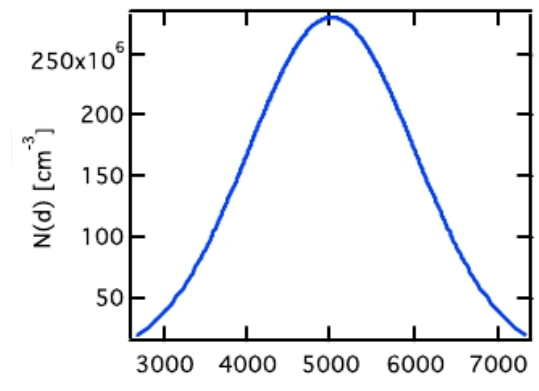
$$= \rho_0 4\pi R^3 \frac{(\sin qR - qR\cos qR)}{(qR)^3}$$

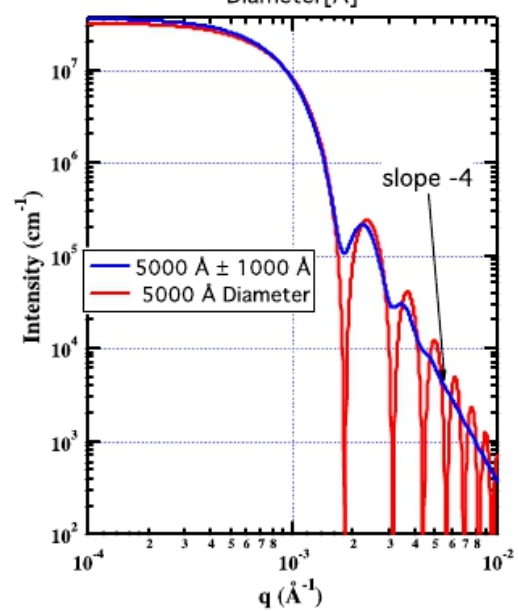
$$= \rho_0 \overbrace{\frac{4\pi R^3}{3}}^{v} \frac{3(\sin qR - qR\cos qR)}{(qR)^3}$$

$$= \rho_0 v \frac{3(\sin qR - qR\cos qR)}{(qR)^3}$$

$$I_N(q) = N\rho_o^2 v^2 \left[\frac{3(\sin qR - qR\cos qR)}{(qR)^3}\right]^2$$







Dale Schaefer, private communications

Form Factor: Scattering from one scatterer

- Assume scatterer is
  - Homogeneous
  - Different density than surroundings

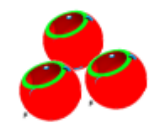
$$\frac{d\Sigma}{d\Omega}(Q) = \left|\Delta\rho\, F(Q,r)\, V(r)\right|^2 = P(Q)$$

- Form factor, *F(Q,r)*, is specific to the shape and size of the scatterers

Spheres:

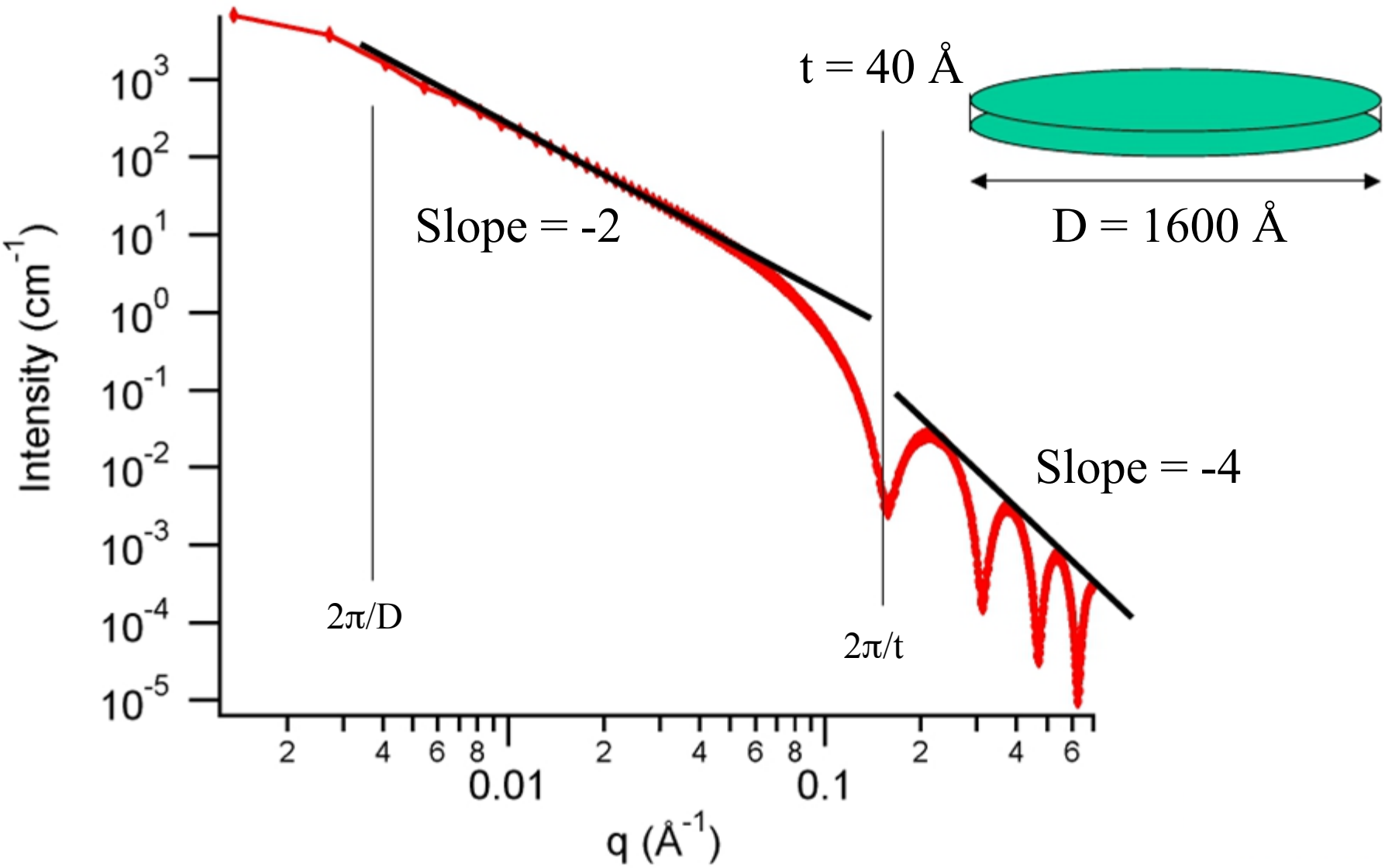
$$F(Q,r) = 3(Qr)^{-3}\left[\sin(Qr) - (Qr)\cos(Qr)\right]$$

Common Form Factors of Particular Shapes

Morphologies	P(q)	Morphologies
Spheres (radius :R)	$\frac{9}{(qR)^6}[\sin(qR) - qR\cdot\cos(qR)]^2 = A_{sph}^2(qR)$	
Spherical shells (outer radius: R_1 inner radius: R_2)	$\frac{[R_1^3\cdot A_{sph}(qR_1) - R_2^3\cdot A_{sph}(qR_2)]^2}{(R_1^3 - R_2^3)^2}$	
Triaxial ellipsoids (semiaxes: a,b,c)	$\int_0^1\int_0^1 A_{sph}^2[q\sqrt{a^2\cos^2(\pi x/2) + b^2\sin^2(\pi x/2)(1-y^2)_1 + c^2y^2}\,]\,dx\,dy$	
Cylinders (radius: R length: L)	$4\int_0^1 \frac{J_1^2[qR\sqrt{1-x^2}\,]}{[qR\sqrt{1-x^2}\,]^2}\,\frac{\sin^2(qLx/2)}{(qLx/2)^2}\,dx$ $J_1(x)$ is the first kind Bessel function of order 1	
Thin disk (radius: R)	By setting L = 0 $\quad \frac{2 - J_1(2qR)/qR}{q^2R^2}$	
Long rod (length: L)	By setting R = 0 $\quad \frac{2}{qL}\int_0^{qL}\frac{\sin(t)}{t}\,dt - \frac{\sin^2(qL/2)}{(qL/2)^2}$	

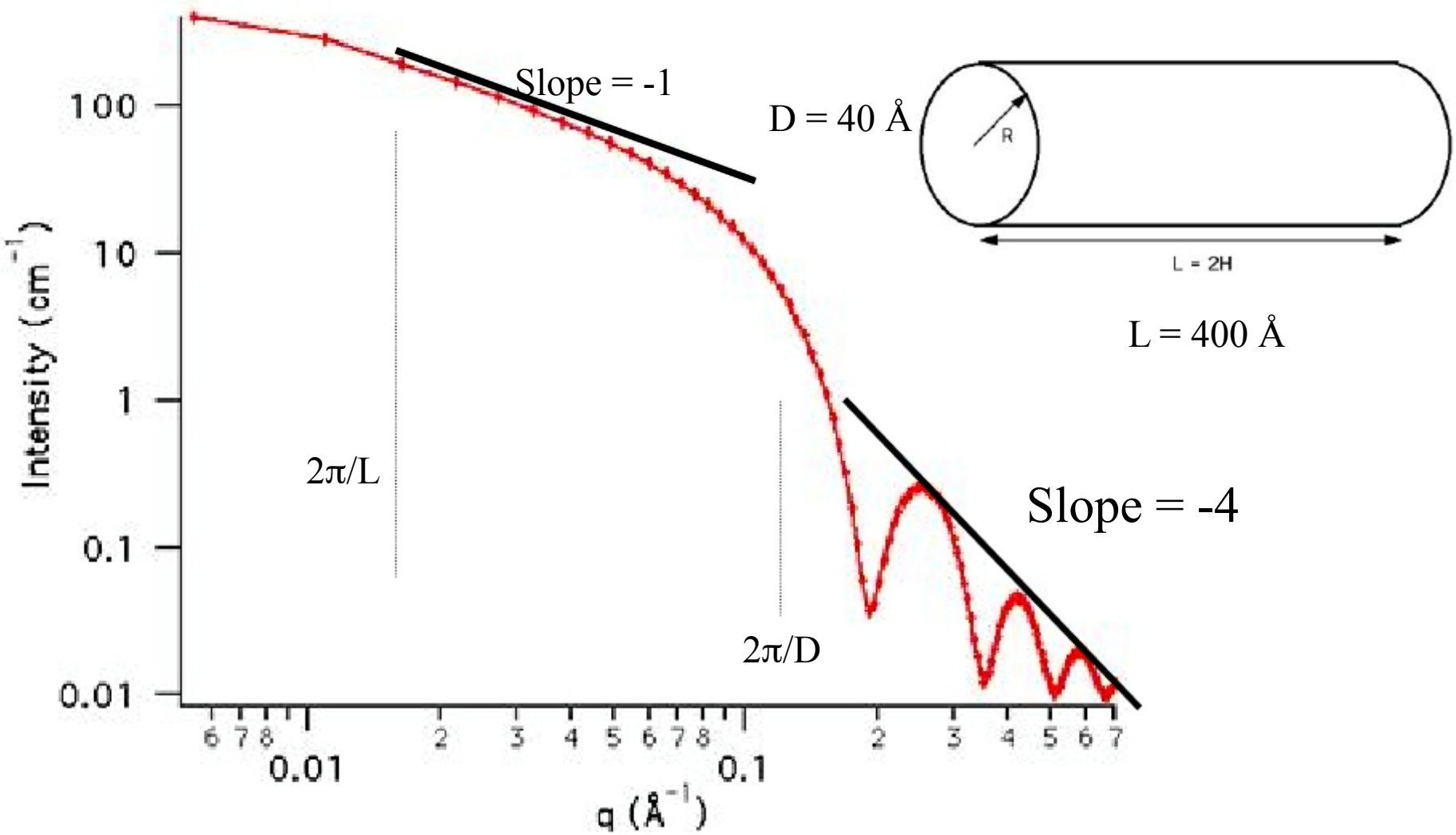
"Structure Analysis by Small Angle X-Ray and Neutron Scattering" L. A. Feigen and D. I. Svergun

Dilute, Randomly-dispersed Disks



Jan Ilavsky, private communications

Dilute, Randomly-dispersed monodisperse Rods



Jan Ilavsky, private communications

Absolute SAS Cross-Section $d\Sigma/d\Omega$

J Appl Cryst **5** (1972) 315-324, **16** (1983) 473-478
Acta Metall Mater **39**.11 (1991) 2477-2487

$$I(Q) = I_0 \, \Omega \, t \, e^{-\mu t} \, \frac{d\Sigma}{d\Omega}(Q)$$

$I(Q)$: intensity, arbitrary units

I_0 : apparent source intensity, arbitrary units

Ω : solid angle subtended by detector

t : sample thickness

μ : linear absorption coefficient

$d\Sigma(Q)/d\Omega$: differential scattering cross-section per unit volume per unit solid angle

Optimal sample thickness

$$I(Q) = I_0\, \Omega\, t\, e^{-\mu t}\, \frac{d\Sigma}{d\Omega}(Q)$$

measured intensity

$$\max\left(\frac{dI}{dt}\right): \quad t = 1/\mu = 0.37$$

Optimal thickness due to absorption

In practice, *I(Q)* can show presence of…

- incoherent scattering background
- multiple scattering

Higher transmissions are typically desired:

- Lower sample thickness, *t*
- Lower absorption, μ (use higher X-ray energy)

Syllabus: Small-Angle Scattering Theory

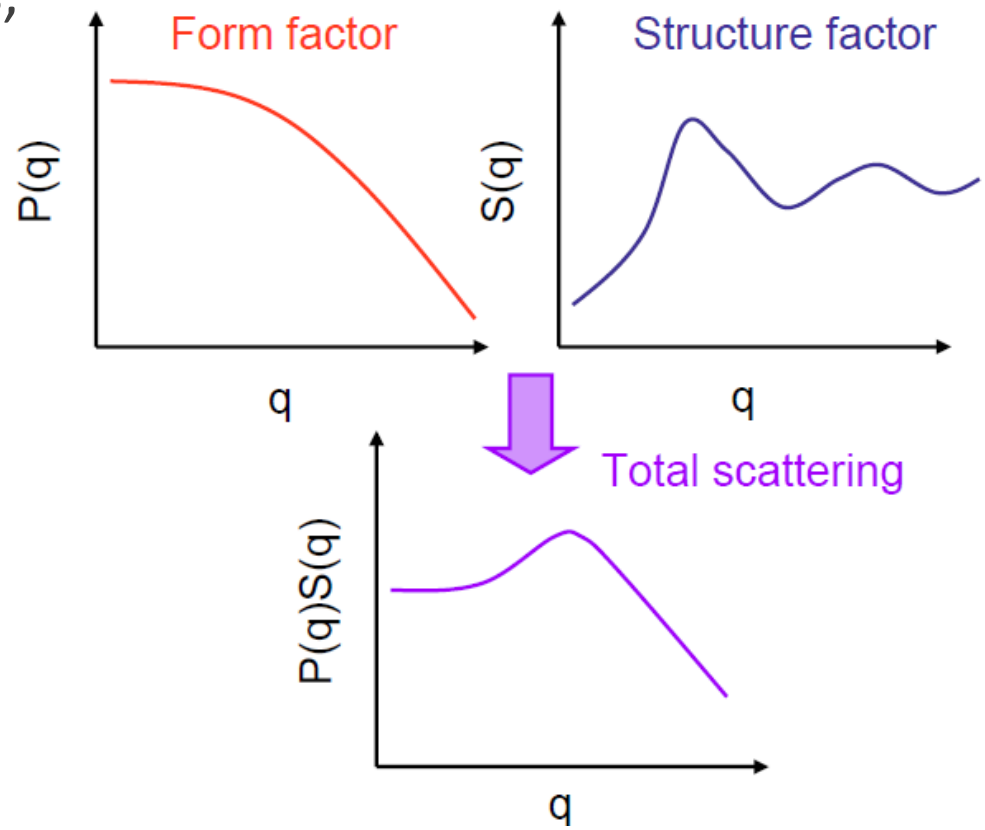
- Why small-angle scattering?
- Basic SAS Theory
  - Scattering length density and Babinet's Principle
  - Radius of gyration
  - Approximations: Invariant, Guinier, and Porod
  - Form Factor
- SAS Theory Beyond R_G
  - Scattering Interference
  - Particle size distributions
  - Contrast variation
  - Fractals
  - Grazing incidence

Structure Factor: common spacing(s) between scatterers

- As concentration increases, these assumptions are removed:
  - [x] Dilute (non-interacting)
  - [x] Randomly dispersed

$$\frac{d\Sigma}{d\Omega}(Q) = P(Q)\,S(Q)$$

- BUT, you ***must*** assume:
  - Monodisperse
  - Common morphology
- Ok in biology
- Not common in materials science



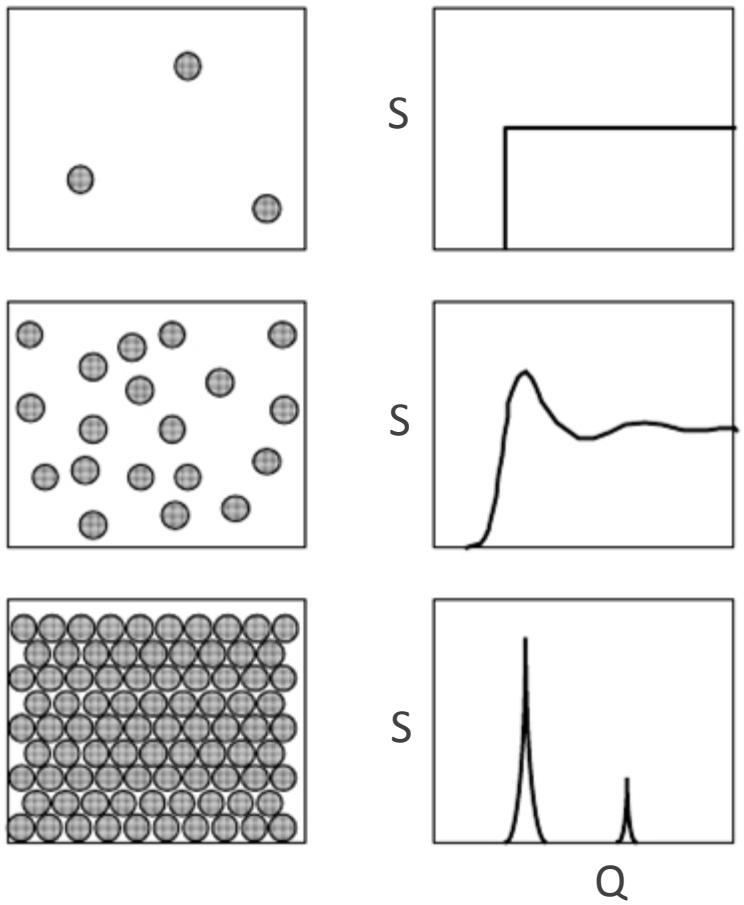
Advances in Colloid and Interface Science 70 (1997) 171-210

S(Q): Concentration effect

Low concentration, gas-like, S(Q)=1

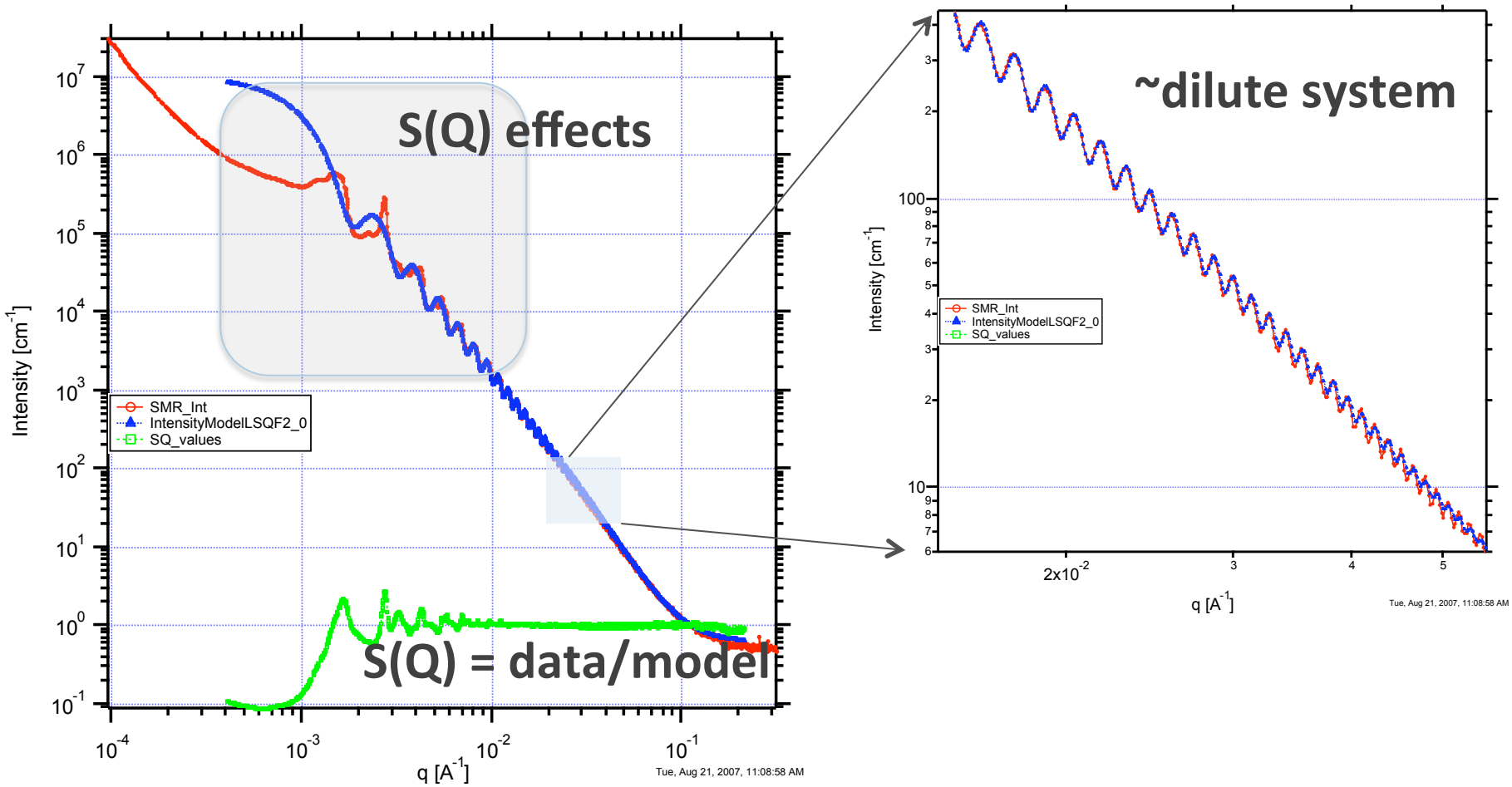
Higher concentration, liquid-like, S(Q) oscillates about 1

High concentration, crystal-like, diffraction peaks



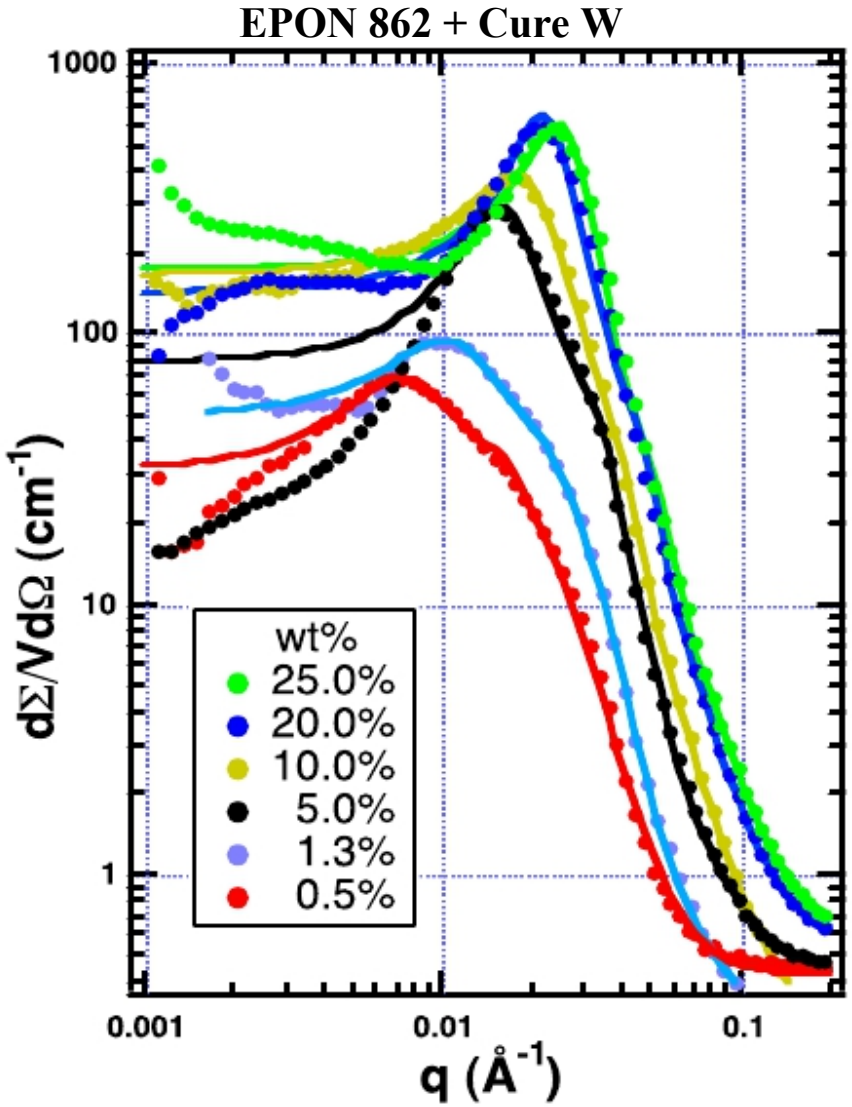
Jan Ilavsky, private communications

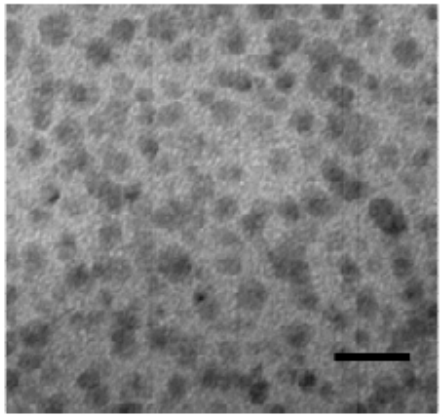
Example data showing structure factor: 1 um spheres, monodisperse, dried powder

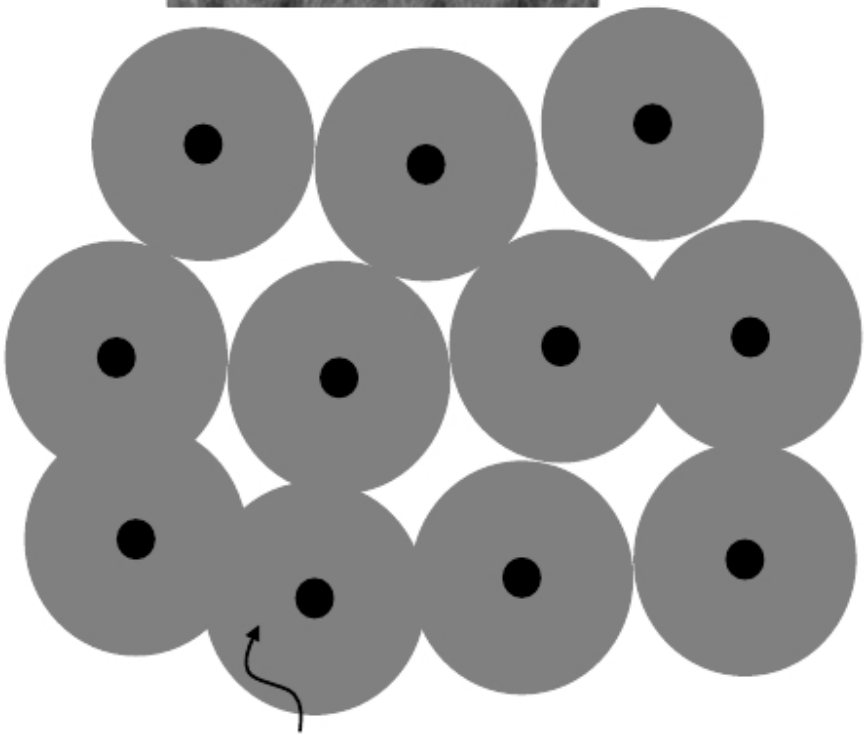


USAXS data – very high q-resolution

Colloidal Silica in Epoxy showing *S(Q)* effects





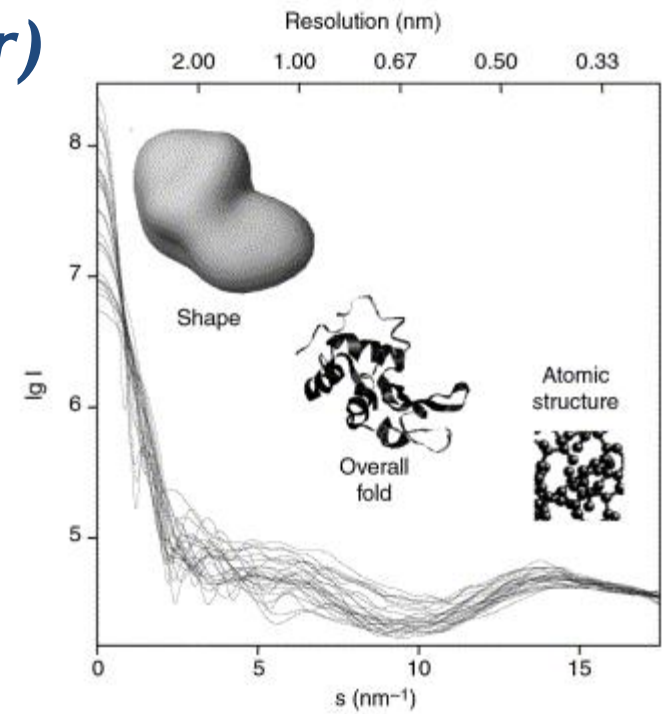


Dale Schaefer, private communications.

Distance Distribution Function: *p(r)*

- Analysis by *p(r)* is often used in biological studies to determine the shape of a protein molecule or in polymer science to study the shapes of colloidal polymers
- An important part of the determination of particle shape is usually the distance distribution function *p(r)*, which may be calculated from the intensity.
- At low and high Q, *p(r)* goes to 0
- The shape of *p(r)* tells something about the shape of the particle. If the function is very symmetric, the particle is also highly symmetric, like a sphere.
- An important assumption in *p(r)* analysis is that polydispersity is negligible.
- D. SVERGUN and M. KOCH, *Small-angle scattering studies of biological macromolecules in solution*, Rep. Prog. Phys. 66.10 (2003) 1735–1782

$$p(r) = \frac{r^2}{2\pi^2}\int_0^\infty I(Q)\frac{\sin(Qr)}{Qr}Q^2\,dQ$$

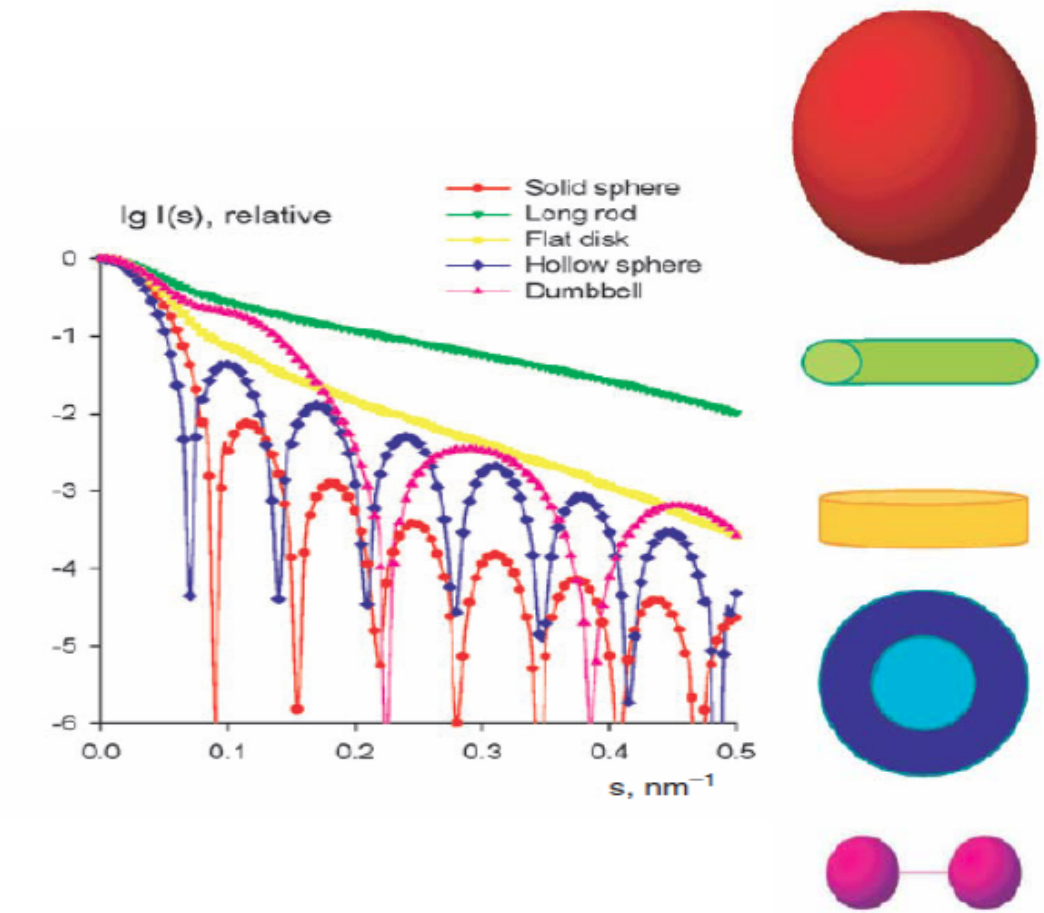


X-ray scattering patterns from proteins with different folds and molecular masses.

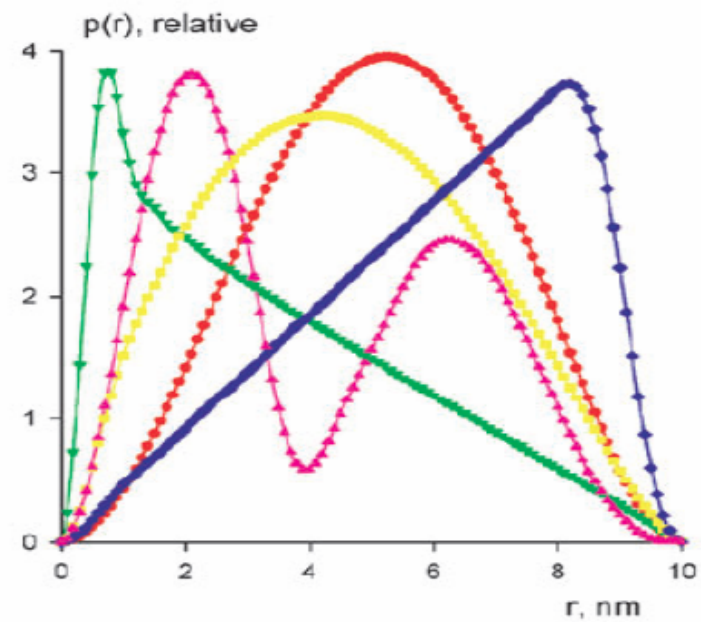
SAS contains information about the gross structural features – shape, quaternary and tertiary structure – but is not suitable for the analysis of the atomic structure.

http://en.wikipedia.org/wiki/Biological_small-angle_X-ray_scattering

Calculated *p(r)* for different particle shapes



Distance distribution function *p*(*r*)



D. SVERGUN and M. KOCH, Rep. Prog. Phys. 66.10 (2003) 1735–1782

Size Distribution Determination

- Useful in materials science investigations

- Assume scatterers are
  - Dilute (non-interacting)
  - Randomly dispersed
  - Same morphology
  - Same contrast, $|\Delta\rho|^2$

$$\frac{d\Sigma}{d\Omega}(Q) = \int_0^\infty \left|\Delta\rho\, F(Q,r)\, V(r)\right|^2 N(r)\, dr$$

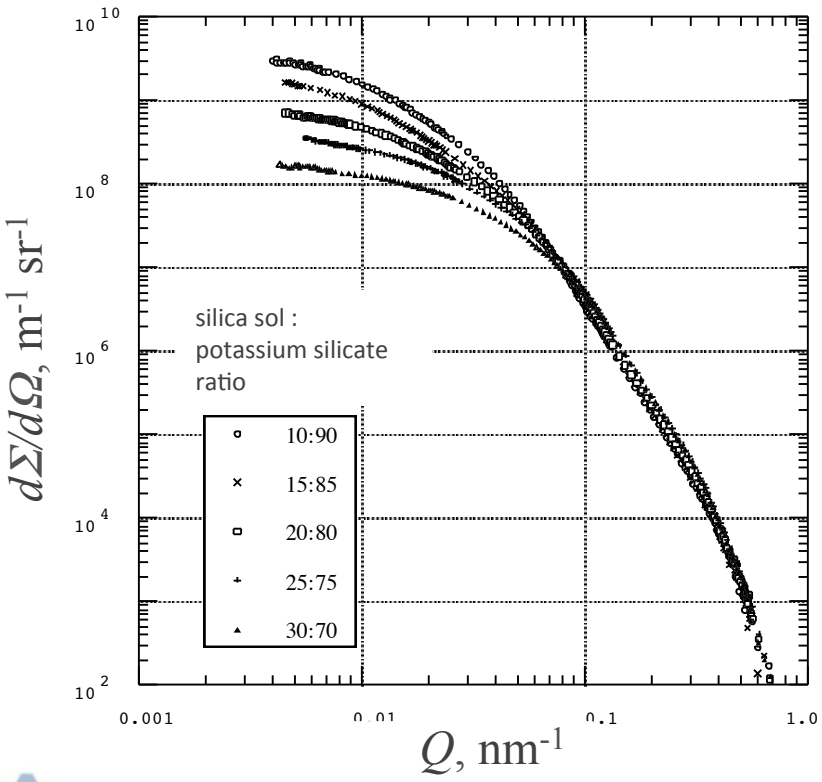
$$\frac{d\Sigma}{d\Omega}(Q) = \left|\Delta\rho\right|^2 \int_0^\infty \left|F(Q,r)\right|^2 V(r) f(r)\, dr$$

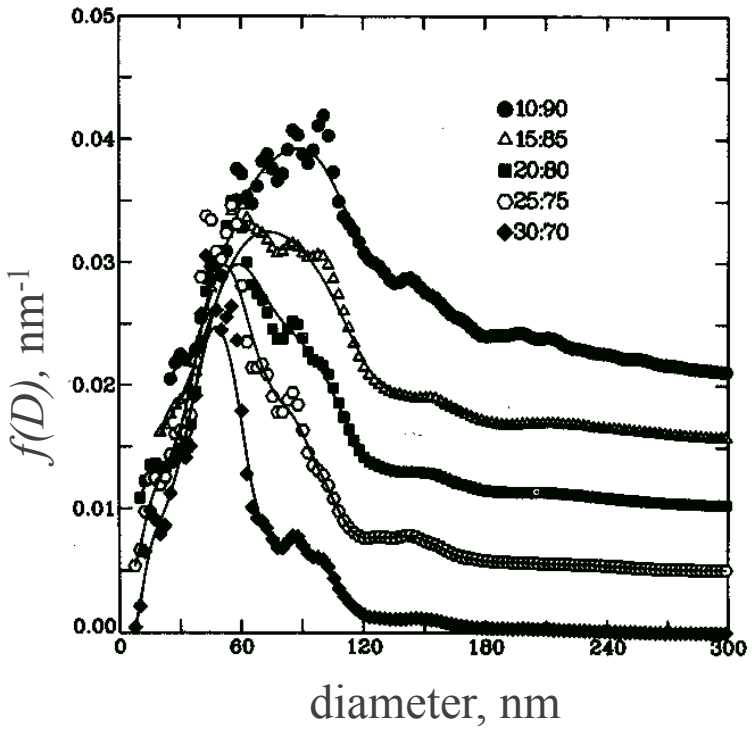
- Not necessary to assume a distribution shape
- Solve for *f(r)* by a regularization method such as:
  - TNNLS: enforcing only positive values of *f(r)*
  - regularization: maximizing smoothness of *f(r)*
  - MaxEnt: maximizing configurational entropy of *f(r)*

P. Jemian, et al.; *Acta Metall Mater* **39**.11 (1991) 2477-2487
J. Skilling and R.K. Bryan; ***Mon Not R Astr Soc* 211** (1984) 111-124.
J.A. Potton, G.J. Daniell, and B.D. Rainford; ***J Appl Cryst* 21** (1988) 891-897, 663-668.

Microporous Silica: determination of size distributions by maximum entropy

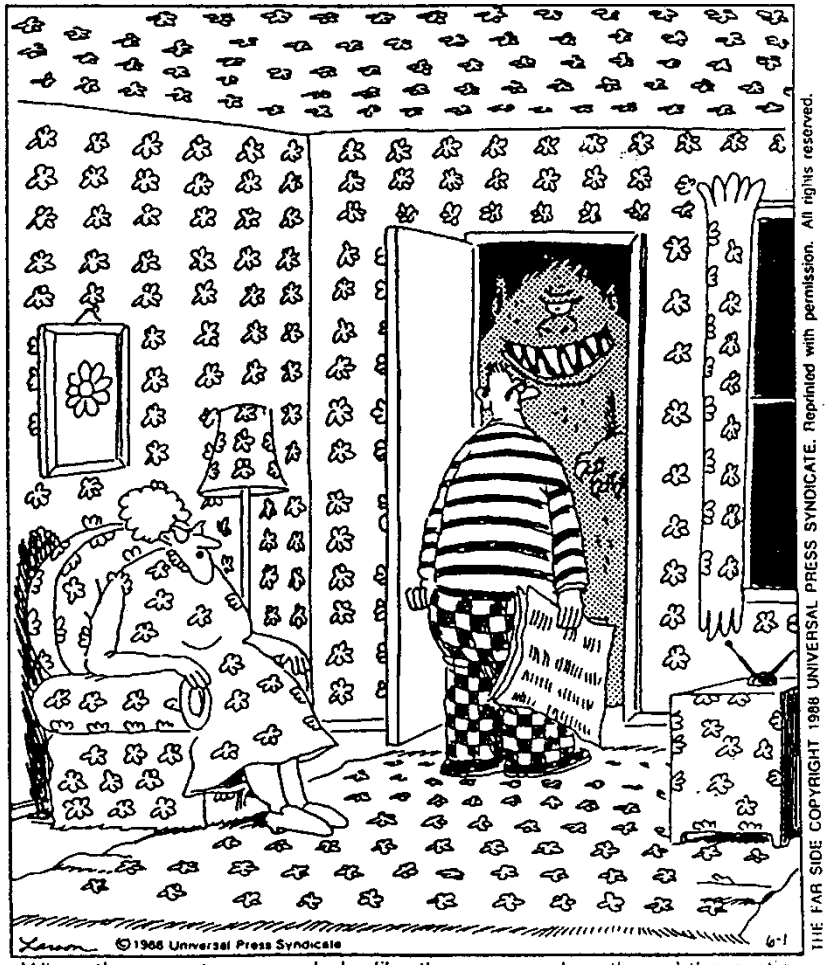
- Mixtures of colloidal silica and potassium silicate, prepared by sol-gel process
- Microstructure: array of particles, small clusters, and aggregates of colloids
- USAXS and SANS to characterize polydisperse size distributions of particles in porous medium as function of mixture ratio





Long, et al., *J Appl Cryst* **23**.6 (1990) 535

Contrast Variation



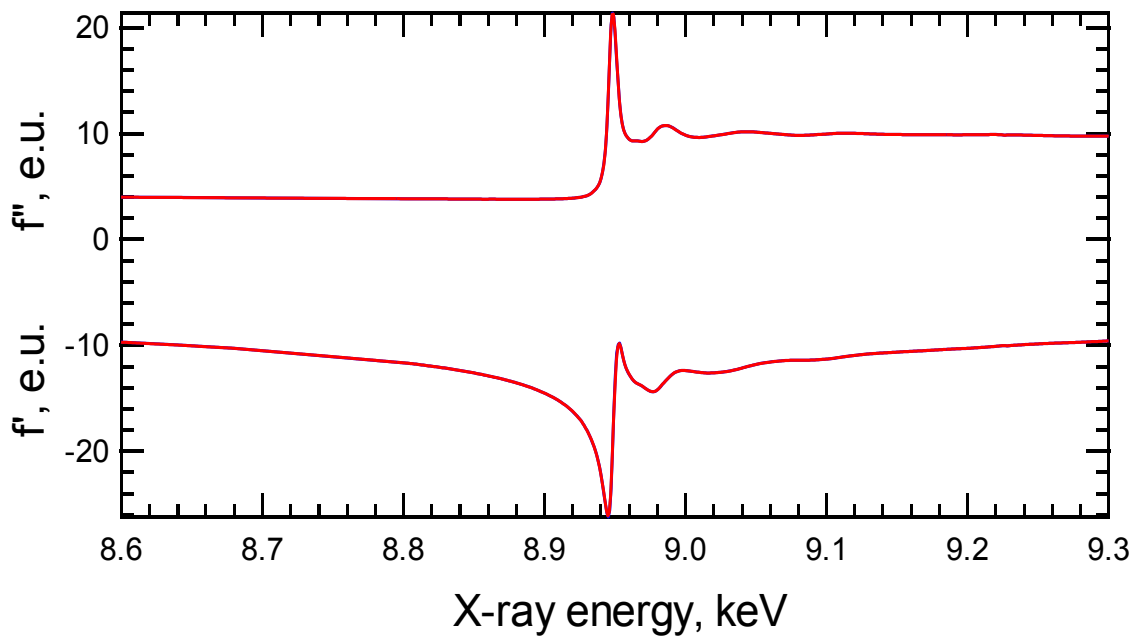
When the monster came, Lola, like the peppered moth and the arctic hare, remained motionless and undetected. Harold, of course, was immediately devoured.

- Needed when more than one type of scatterer is present
- Vary $|\Delta\rho|^2$ of one type, holding others constant

- Anomalous scattering (X-ray & neutron)
- Isotope substitution (neutron)
- Isomorphous replacement
- Magnetic scattering (neutron)
- Concentration variation (X-ray & neutron)
- ...

Anomalous Small-Angle X-ray Scattering

- Why anomalous SAXS?
  - Element-specific contrast variation
  - Use to separate population distributions of scatterers
- Will ASAXS solve every problem?
  - Not even close
  - The easy problems are already taken



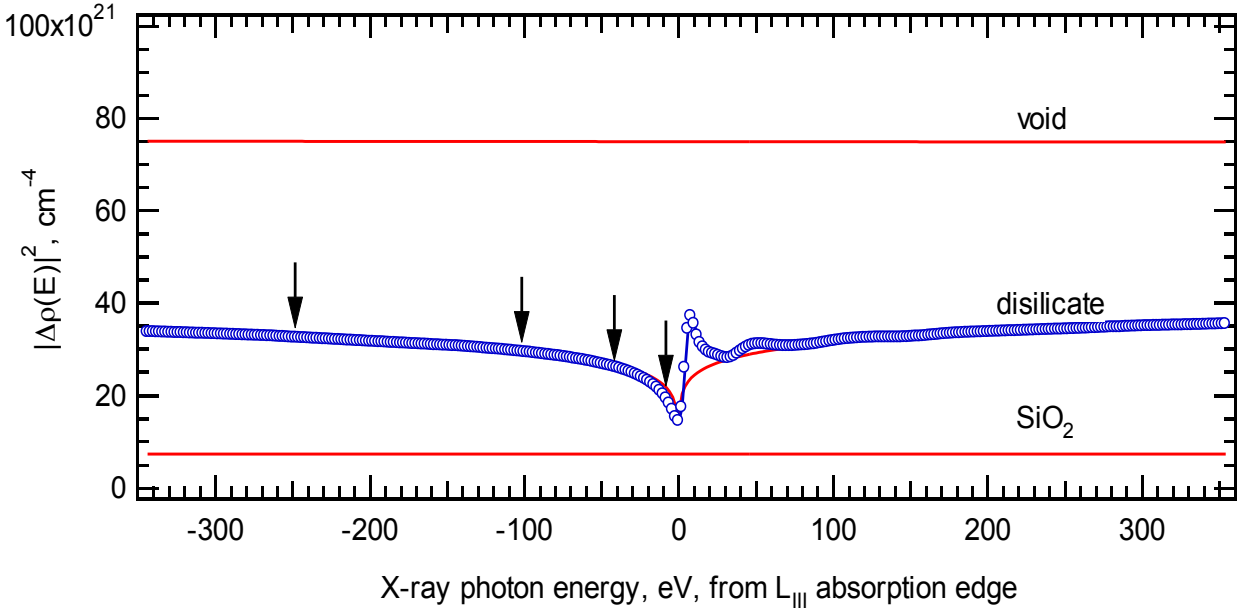
Anomalous dispersion terms of Yb in SN-88 near the Yb L_{III} edge (8.939 keV)

X-ray photon Energy selection for ASAXS contrast variation study

Calculate the scattering contrast of the major populations
Choose energies so that $|\Delta\rho(E)|^2$ are evenly-spaced

$$\Delta\rho_k(E) = r_e(E)\sum_Z \Delta c_Z\left[Z + f'_Z(E) + if''_Z(E)\right]$$

X-ray scattering contrast of scatterers in SN-88 near the Yb L_{III} edge



ASAXS: the gradient method

scattering vector magnitude

$$Q = (4\pi/\lambda)\sin\theta$$

intensity of scattering

$$I(Q,E) = \frac{d\Sigma}{d\Omega}(Q,E) = \sum_k |\Delta\rho_k(E)|^2 \int_0^\infty f_k(D)\ V(D)\ |F(Q,D)|^2\ dD$$

intensity, simplified

$$I(Q,E) = \int_0^\infty \varphi(D,E)\ G(Q,D)\ dD$$

Solve for *φ(D,E)* with MaxEnt, regularization, or some other constrained method.
For example, *J Appl Cryst* **21**.6 (1988) 663-668.

Use scattering contrast to separate *f(D)* for each population

$$\varphi(D,E) = |\Delta\rho_{anomalous}(E)|^2\ f_{anomalous}(D) + |\Delta\rho_{fixed}|^2\ f_{fixed}(D)$$

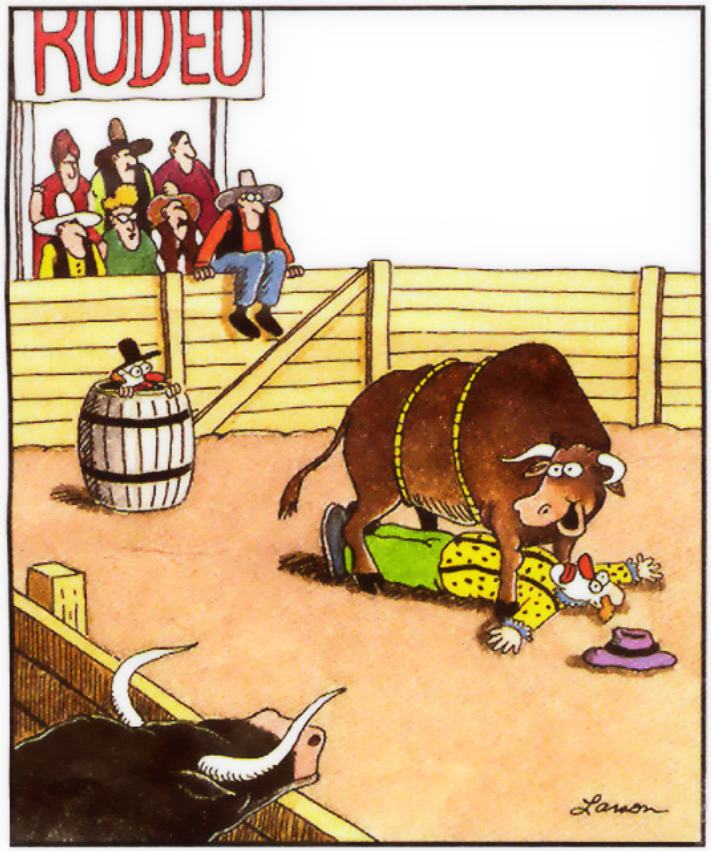
ASAXS Examples

ASAXS is definitely not a panacea technique

Tough to find systems with significant contrast and volume fraction

Measurements are tedious and must use absolute intensity

Instrument must be free of artefacts

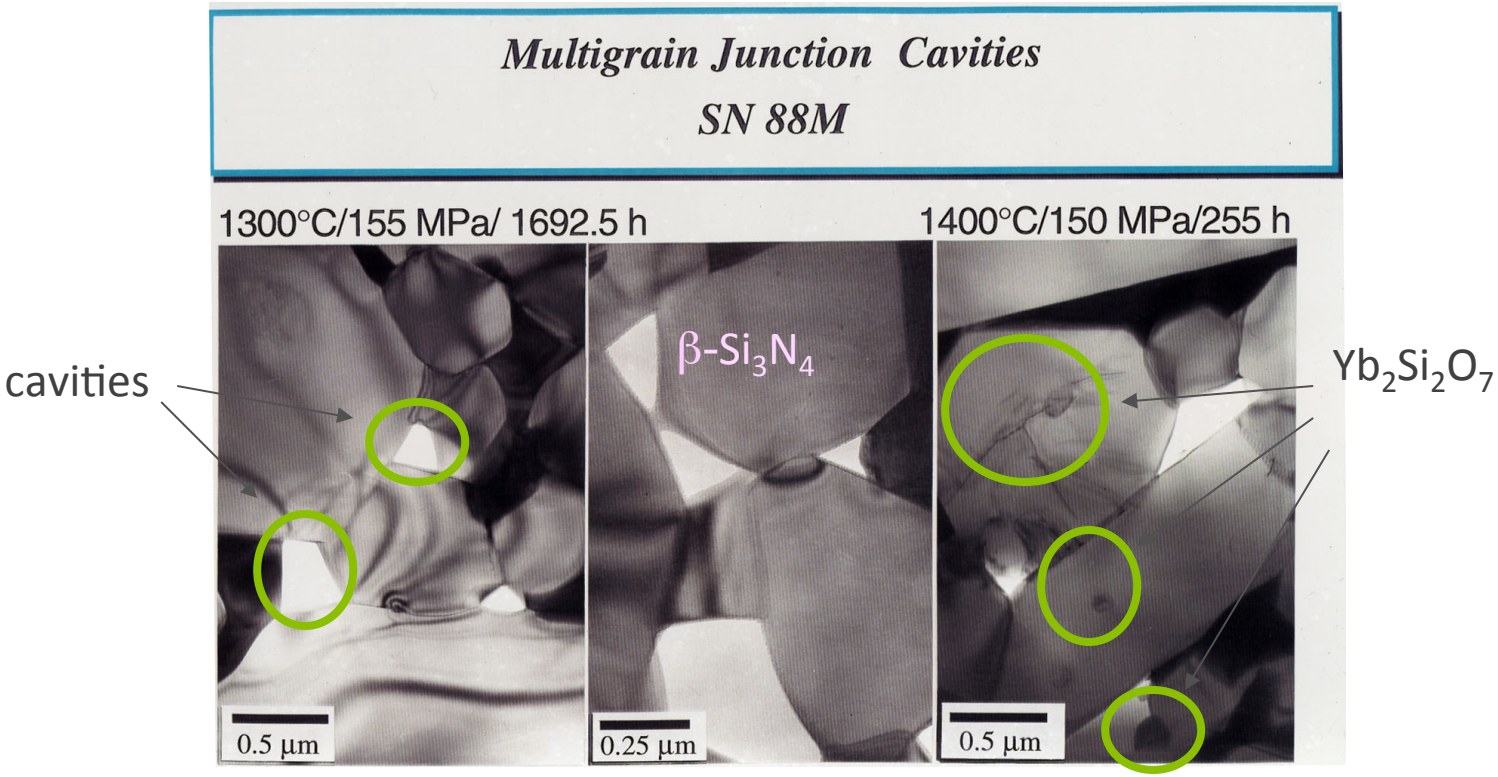


"Hey! I got one! I got one!"

© United Press International, Gary Larson, *The Far Side*.

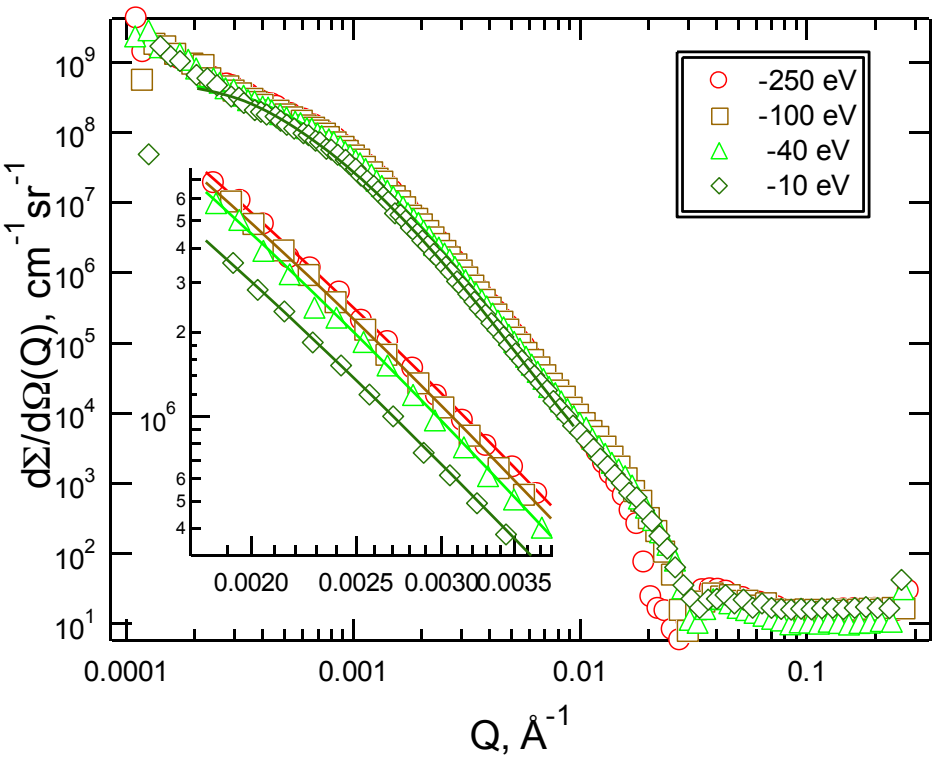
Note, "I got one! I got one!" … that makes two examples

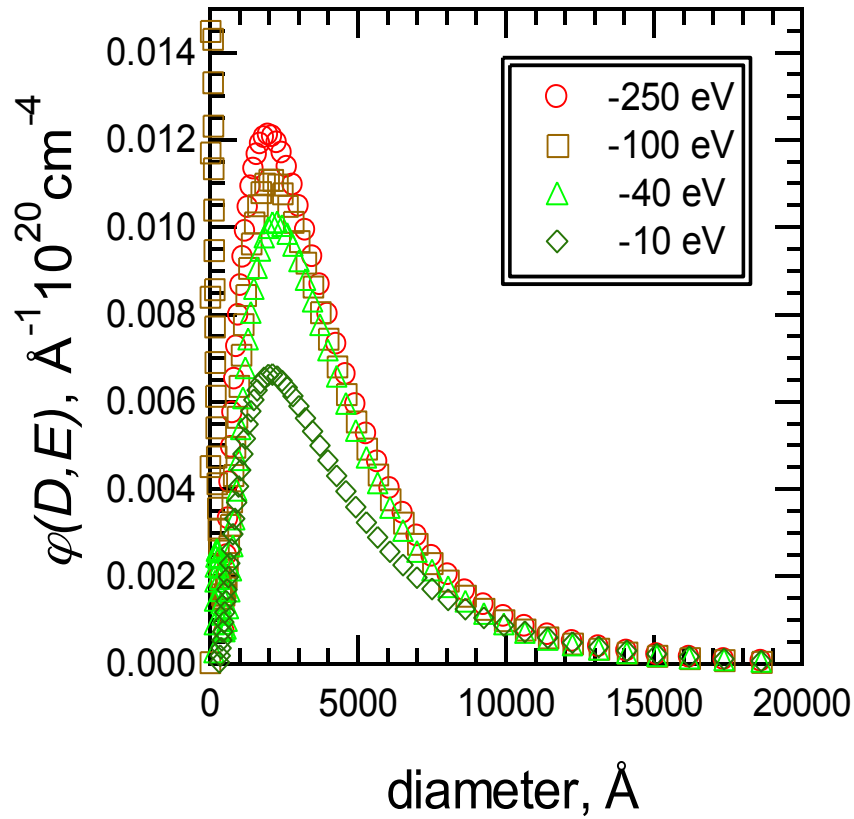
ASAXS Example #1: Tensile Creep Resistance of Commercial Silicon Nitride



- commercial grade of gas-pressure sintered silicon nitride (designated SN88)
- β-Si_3N_4 grains
- major crystalline secondary phase after heat treatment is ytterbium disilicate, $Yb_2Si_2O_7$
- minor phases include residual $Yb_4Si_2N_2O_7$, $Y_5Si_3NO_{12}$, residual SiO_2 glass, and porosity

A-USAXS near the Yb L_{III} edge from SN-88 tensile creep sample, 50 h

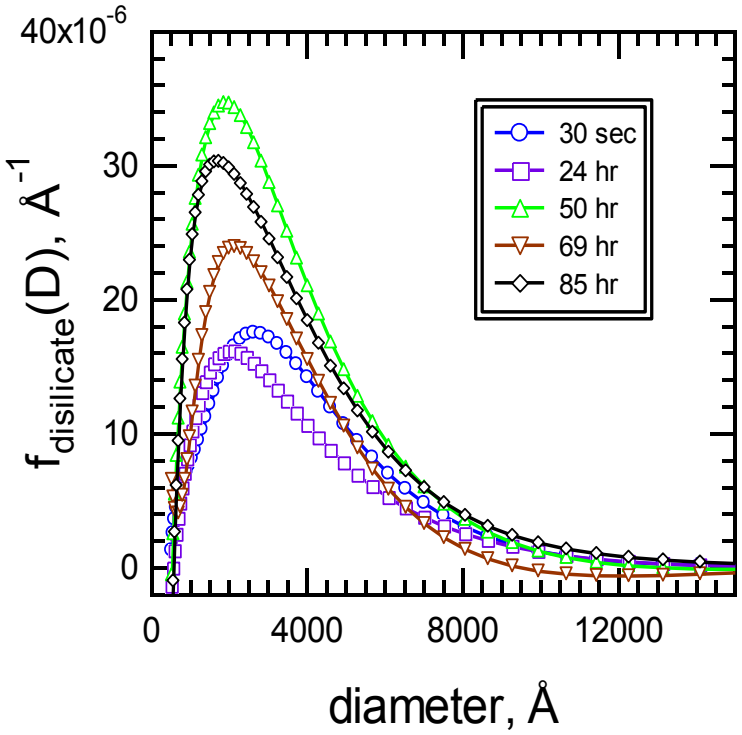




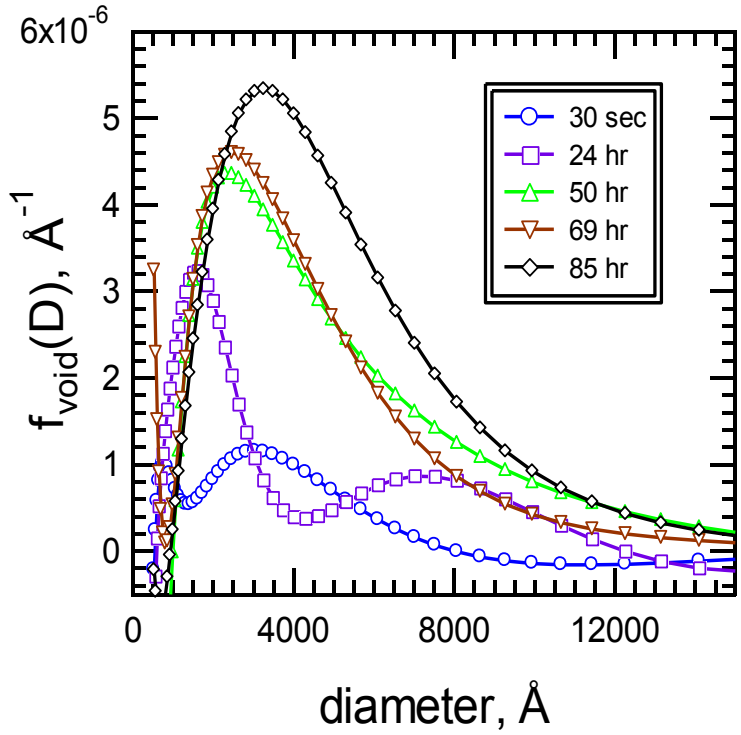
Lofaj, Wiederhorn, Long, Hockey, Jemian, Browder, Andreasen, & Taffner; ***J Euro Ceram Soc* 22** (2002) 2479-2487.

Evolution of size distributions in SN-88 with test time, 1400 C

Yb disilicate size distributions, grip section

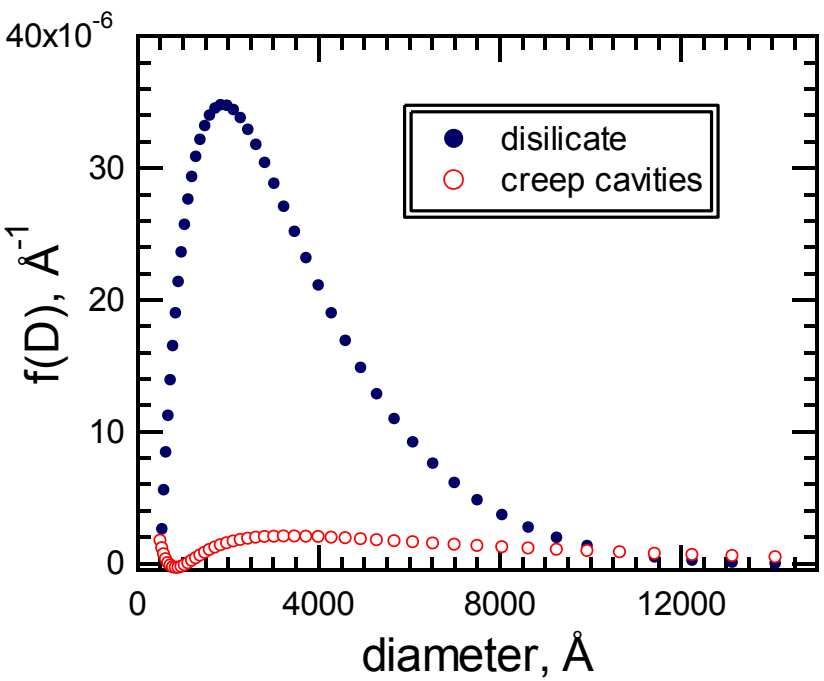


tensile creep cavity size distributions

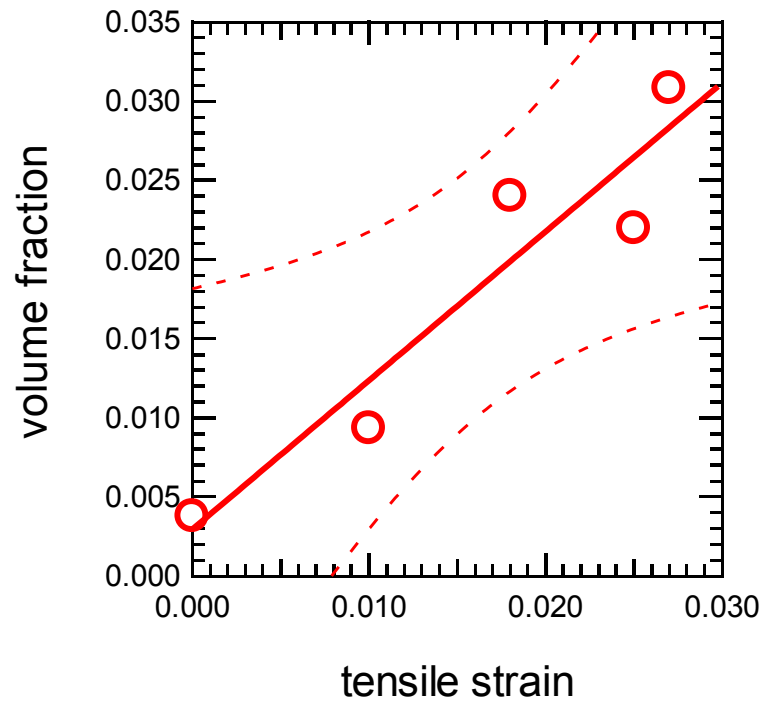


Lofaj, Wiederhorn, Long, Hockey, Jemian, Browder, Andreasen, & Taffner;
***J Euro Ceram Soc* 22** (2002) 2479-2487.

Tensile Creep Resistance of Commercial Silicon Nitride: A-USAXS Results



Creep pore size distribution separated from size dist of secondary phase pockets of comparable size.



Linear relationship between *Vv* measured from A-USAXS and tensile strain agrees well with density change data and confirms that cavitation is the main creep mechanism.

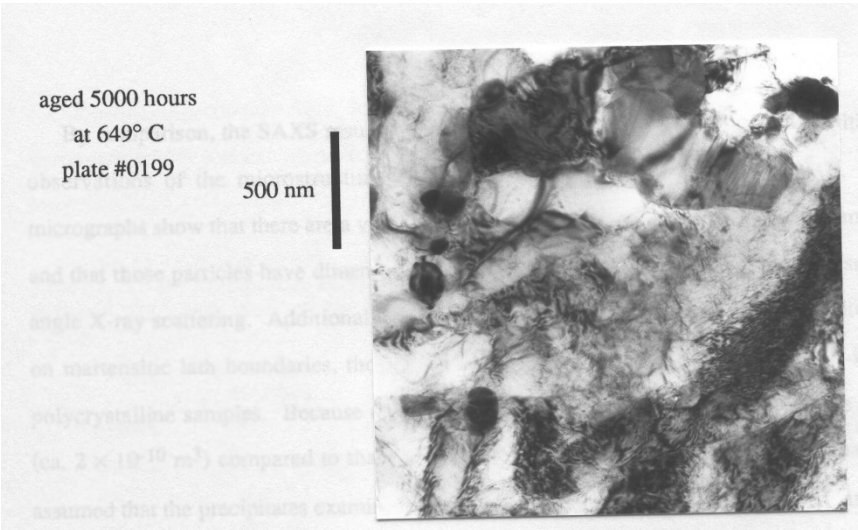
Lofaj, Wiederhorn, Long, Hockey, Jemian, Browder, Andreasen, & Taffner; ***J Euro Ceram Soc* 22** (2002) 2479-2487.

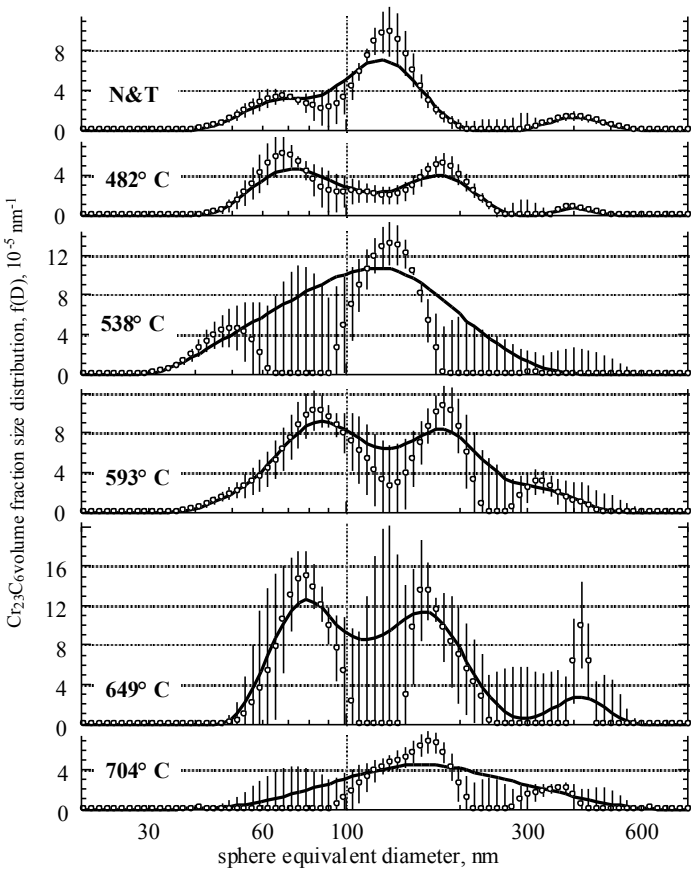
ASAXS Example #2: Stability of Modified Fe9Cr1Mo Steel at High Service Temperatures

- Ferritic steel developed at ORNL (1983), proposed for use in power-generation at elevated temperatures
- Attractive properties
  - High temperature use in corrosive environments
  - high rupture strength at both room and elevated temperatures
  - good weldability
  - low thermal expansion
  - resistance to radiation-induced void swelling
- $Cr_{23}C_6$, VC, and NbC present
- Isolate the $Cr_{23}C_6$ population by ASAXS

P. Jemian, et al.; *Acta Metall Mater* **39**.11 (1991) 2477-2487

Chromium Carbide Distribution in Modified Fe9Cr1Mo steel by ASAXS





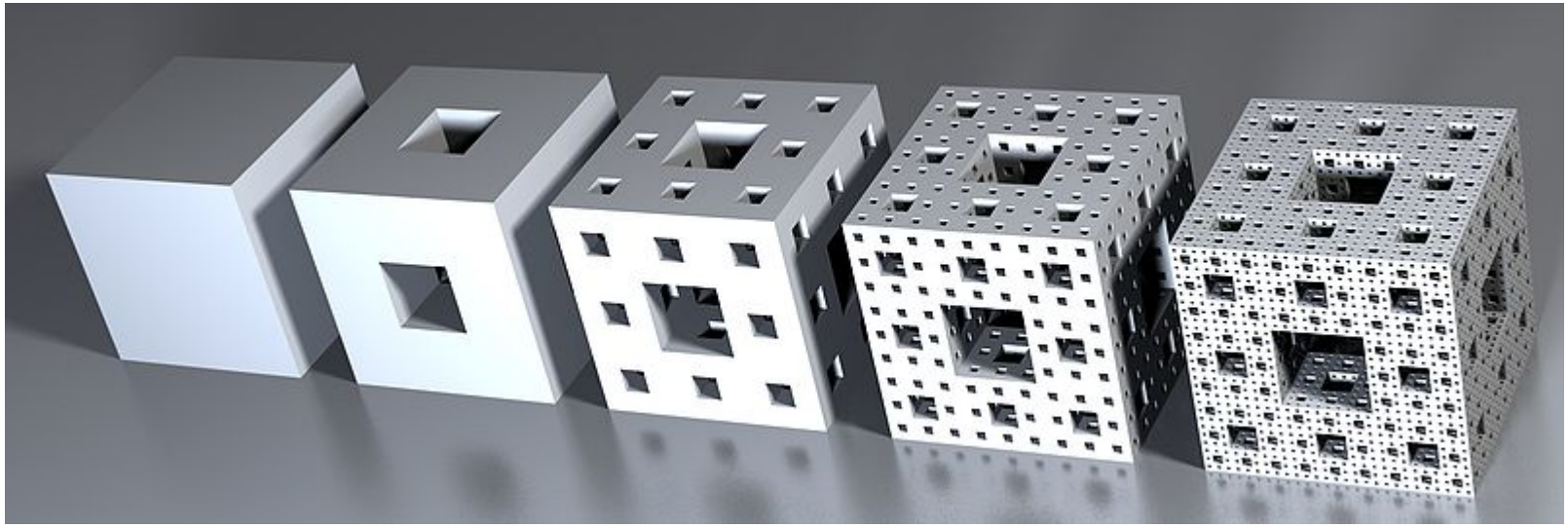
Volume-fraction size distributions of $Cr_{23}C_6$ in Modified Fe9Cr1Mo steel, determined by the ASAXS gradient method. The vertical bars represent the margin of error. The solid line is spline smoothed.

Jemian, Ph.D. Thesis, 1990,Northwestern

Fractals

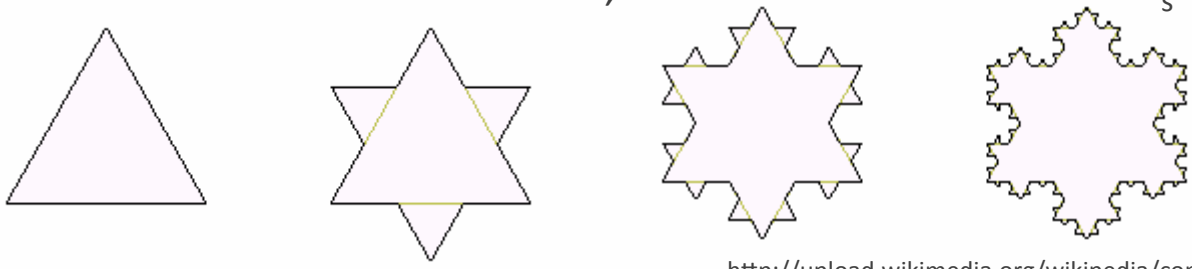
- fractal objects present the same structure on any length scale

Mass fractal: Menger sponge, mass fractal dimension $D_m = 2.72$



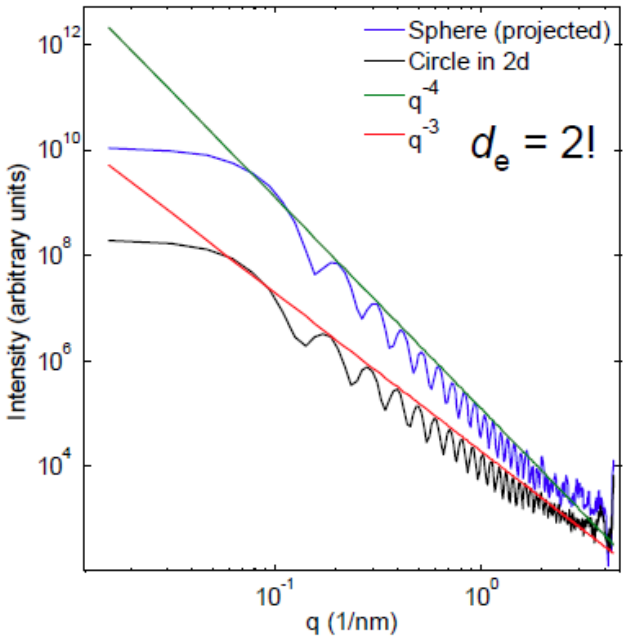
http://commons.wikimedia.org/wiki/File:Menger-Schwamm-Reihe.jpg

Surface fractal: Koch snowflake, surface fractal dimension $D_s = 1.26$ (in $d_e = 2$)



http://upload.wikimedia.org/wikipedia/commons/8/8e/KochFlake.png

Fractals in small-angle scattering: power law analysis of *I(Q)*



Many SAXS curves follow a power law

$$I(q) \propto q^{-\alpha}$$

Mass fractal:
$\alpha = D_m$ (0 – 3)

Surface fractal:
$\alpha = 2d_e - D_s$ ($6 - D_s$, when $d_e = 3$)

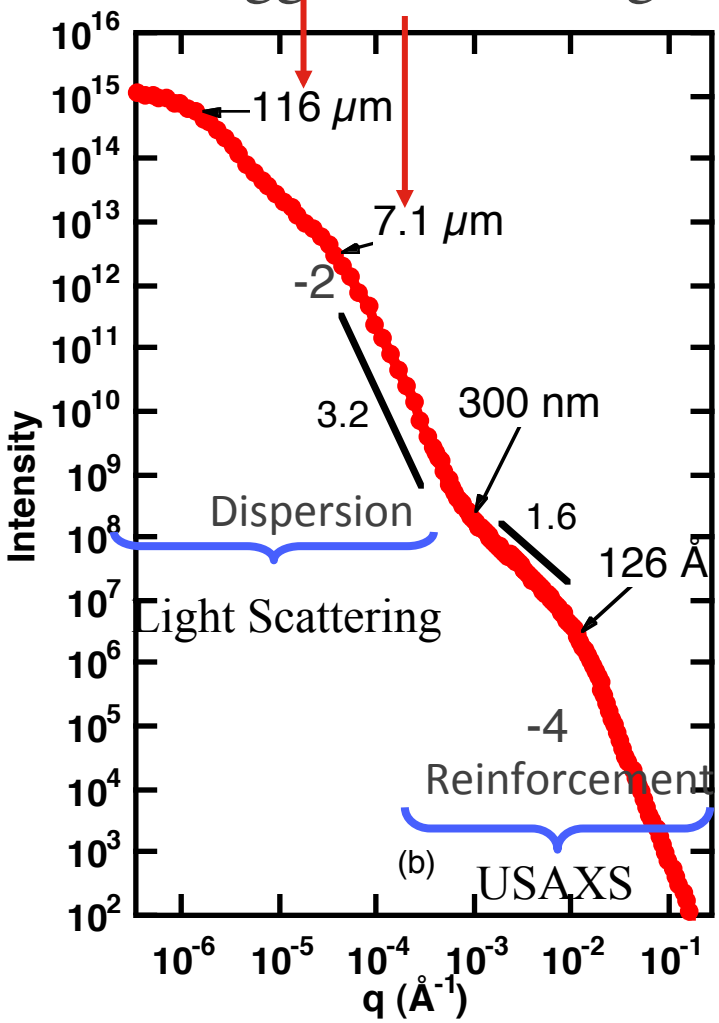
Shape	D_m	D_s	
Line	1	0	
Platelet	2	1	
Sphere	3	2	**Porod law**
			$I(q) \propto q^{-4}$

D_m = mass fractal dimension
D_s = surface fractal dimension
d_e = Euclidian dimension (3 in real life)

source: U. Vainio; 2010 DESY summer school lectures

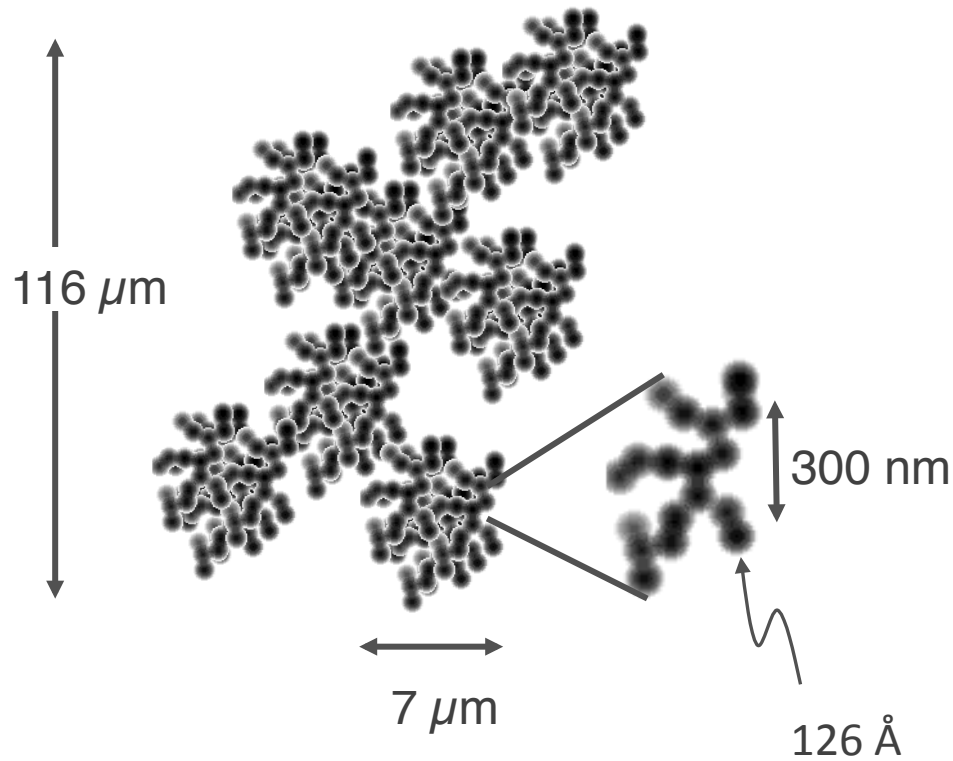
Morphology of Dimosil® Tire-Tread Silica

Two Agglomerate length Scales



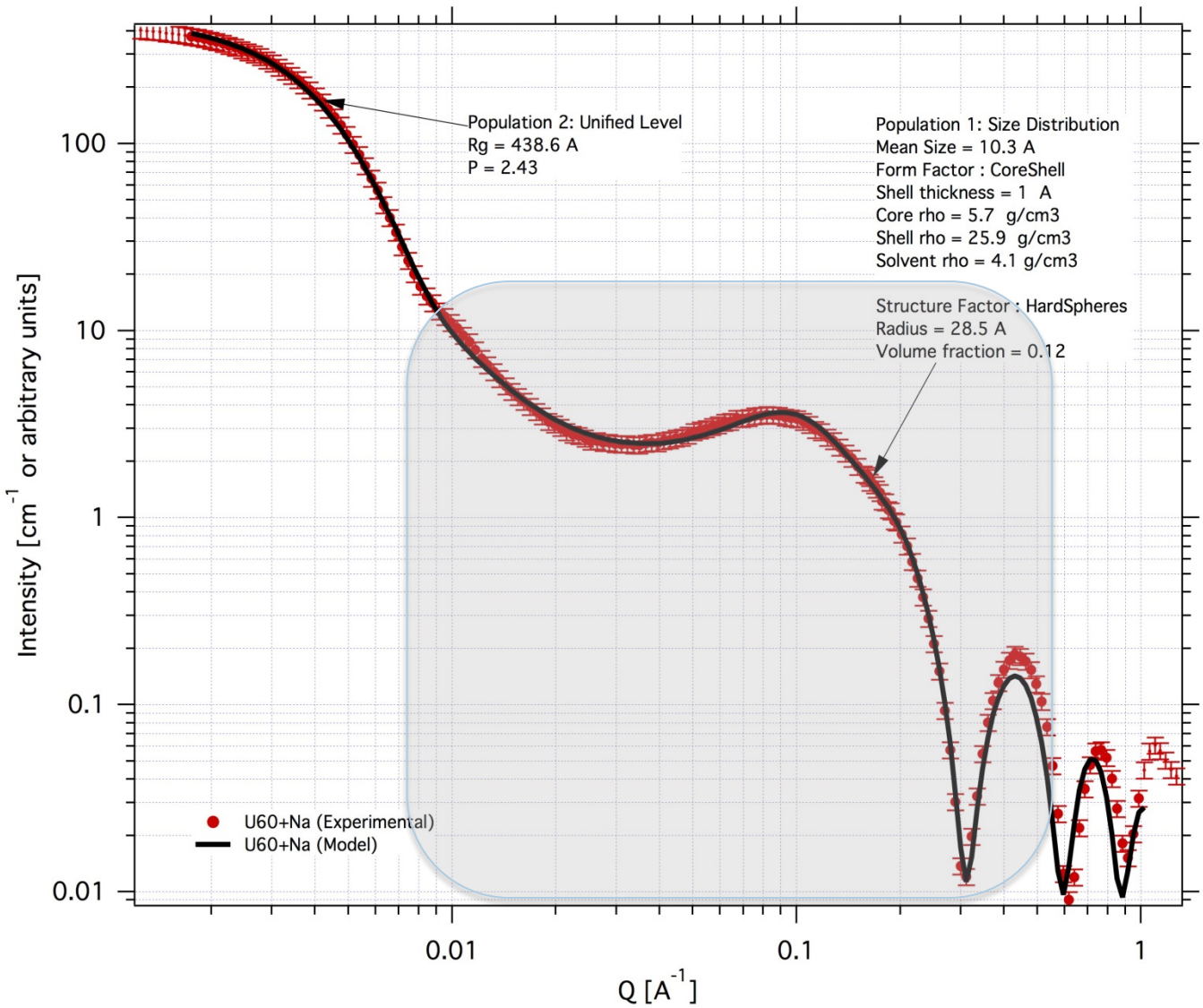
Soft = Chemically Bonded

Hard = Physically Bonded



Dale Schaefer, private communications.

U_{60} aggregates: complex analysis



U_{60} aggregates after 8 hour aggregation induced by addition of Group I cations (Li, Na, K,..).

Peter Burns group, U Notre Dame, IN

Whole graph – USAXS&SAXS combined

Shaded area – typical SAXS/SANS

Jan Ilavsky, private communications

Wrap up: SAS Theory and Applications

- SAS investigations measure nanoscale structure
- Many different materials of technological importance can be investigated
- Contrast variation methods possible
- Statistically significant results
- Unique results not obtainable by other methods
- Complementary methods increase the information content which can be realized from a quantitative SAS investigation