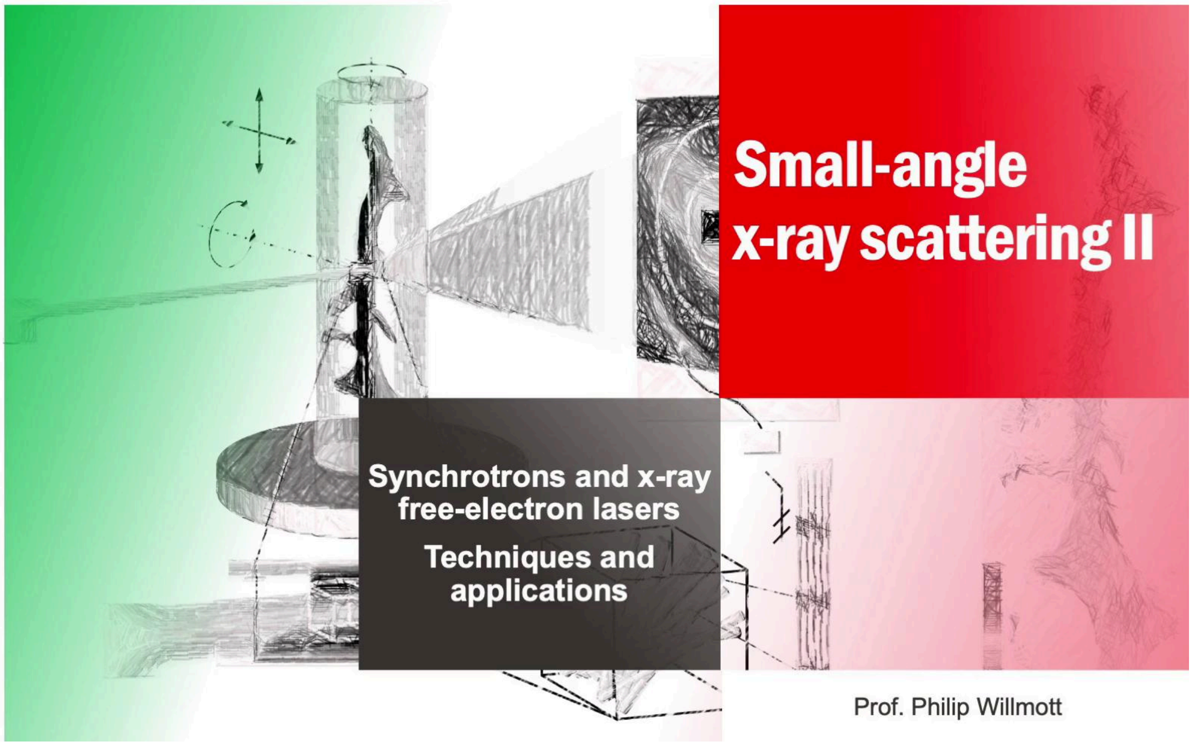
EPFL

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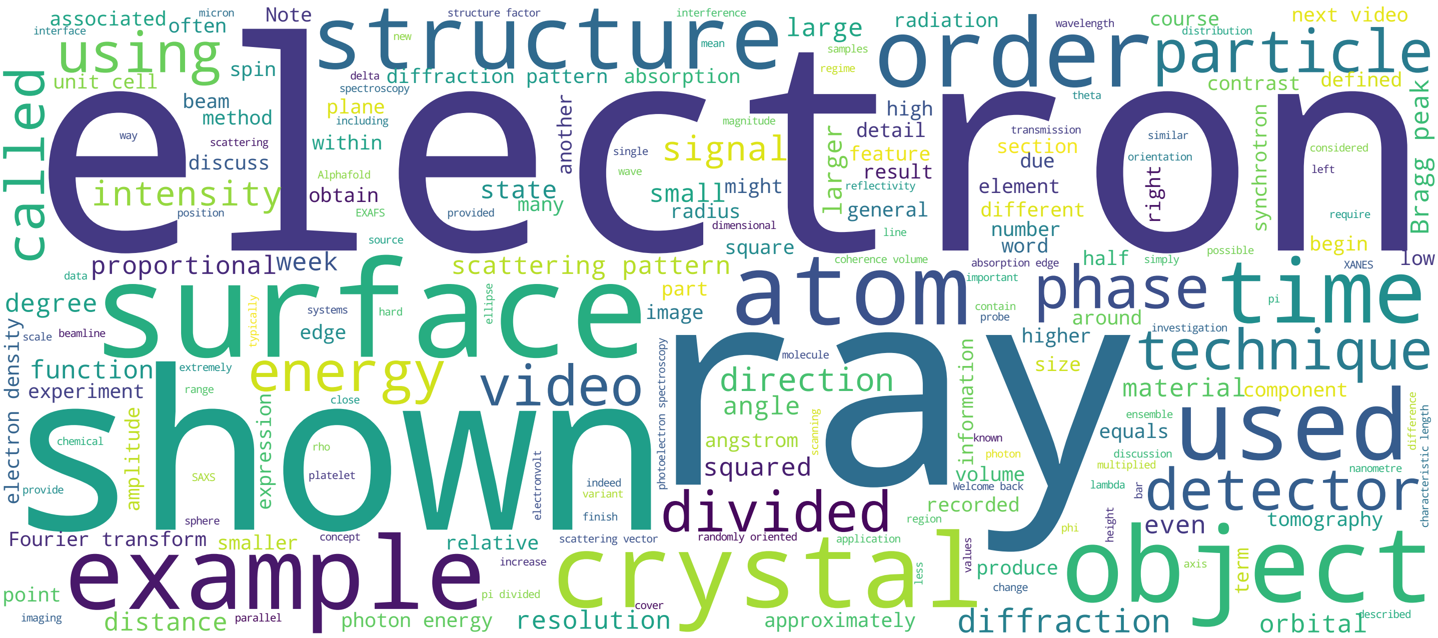



Search MOOC

Video

EPFL

# Contents and objectives of this video

- Q-regimes
- Simple idealized shapes
- Scattering curves for different shapes

In this video, we begin by considering different scattering regimes. In particular, those in which the scattering vector Q is much smaller than two pi upon D, where D is a characteristic length of the object under investigation, and conversely, those in which Q is much larger than two pi divided by D. As we will see, some simplifications can be made in these limiting cases We will then consider the scattering patterns produced by simple idealized shapes, such as spheres, ellipsoids, rods, and platelets.

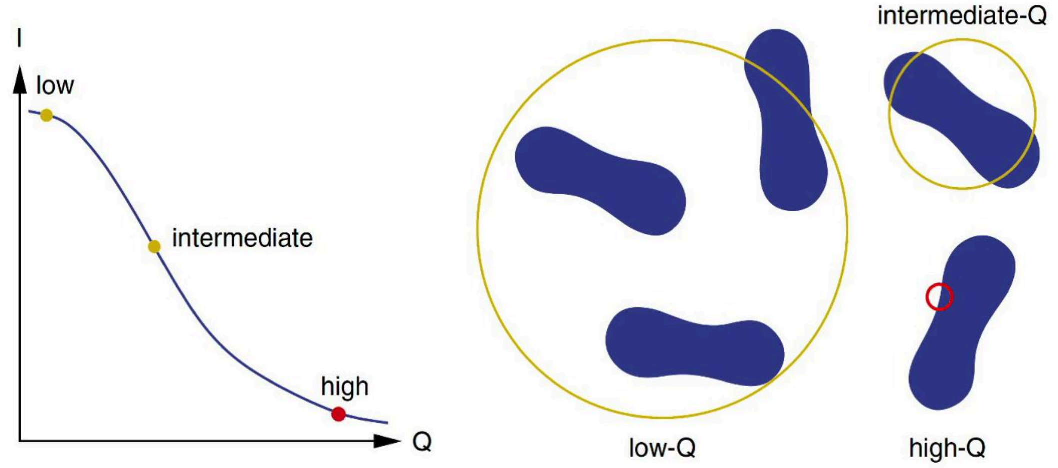
Notes

Summary

0m 05s

# Q-regimes and what they're good for

- For a given Q, resolution = $2\pi/Q$
- High Q
  - Probes surface/interface where there are changes in electron density
  - "Porod" regime



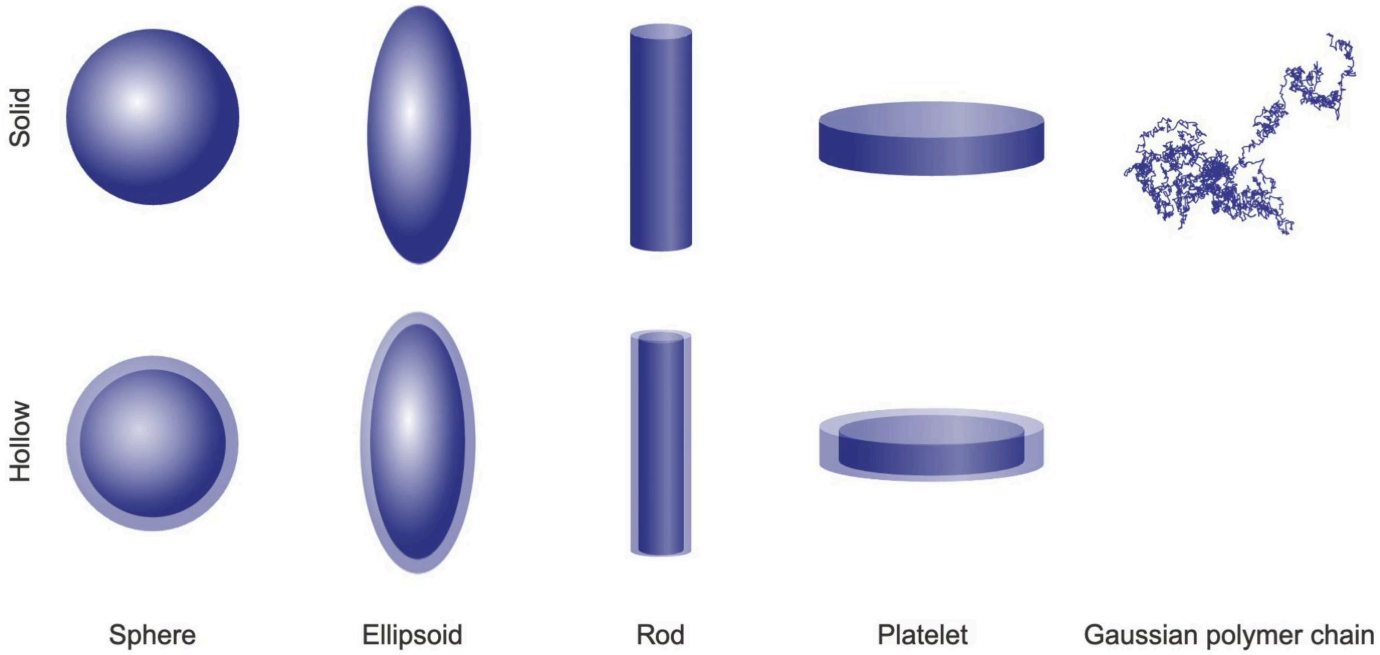

The resolution of a scattering experiment is given by D equals two pi divided by Q. The larger is Q, the smaller the features that can be resolved. In the low Q regime, or the so-called Guinier regime, fine details of the objects under investigation are inaccessible, and only the general extent of the object can be ascertained. In contrast, in the high Q or Porod regime, the surface of the object or interfaces between components of that object with differing electron density are probed. The intermediate regime can provide information on fractal scaling in systems with nested characteristic length scales. We consider these regimes in more detail in the following video.

Notes

Summary

0m 40s

# Idealized shapes of particular interest



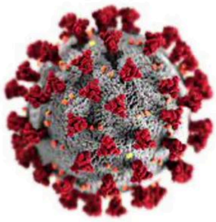

In this section, we will consider the scattering patterns produced by some idealized geometrical objects, such as hollow or solid spheres, ellipsoids, rods, platelets, and loose randomly folded polymer chains.

Notes

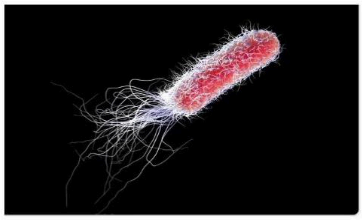
Summary

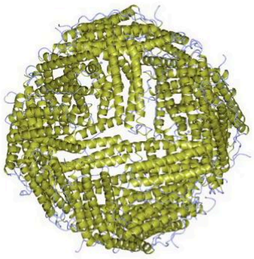
1m 37s

# Idealized shapes of particular interest

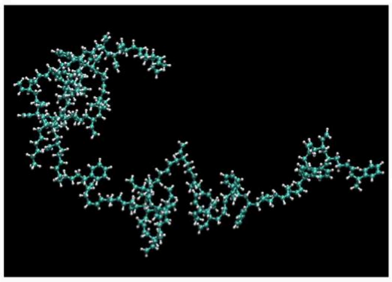

COVID-19 virus


Paramecium


Bacillus bacterium


Apoferritin protein


Red blood cells


Styrene-butadiene copolymer chain



These are considered as real objects can often be closely approximated by them.

Notes

Summary

1m 55s

# Scattering curves – general comments

$$I(Q) = \underbrace{N}_{\text{Number density of particles}} \underbrace{V^2}_{\text{Volume of particle}} \underbrace{(\Delta\rho)^2}_{\text{Electron-density contrast of particle}} [\underbrace{\mathcal{F}(Q)}_{\text{Form factor of particle}} \underbrace{\overset{\simeq 1}{\cancel{\mathcal{S}(Q)}}}_{\text{Coherence factor}}]^2 + \underbrace{B}_{\text{Background signal}}$$

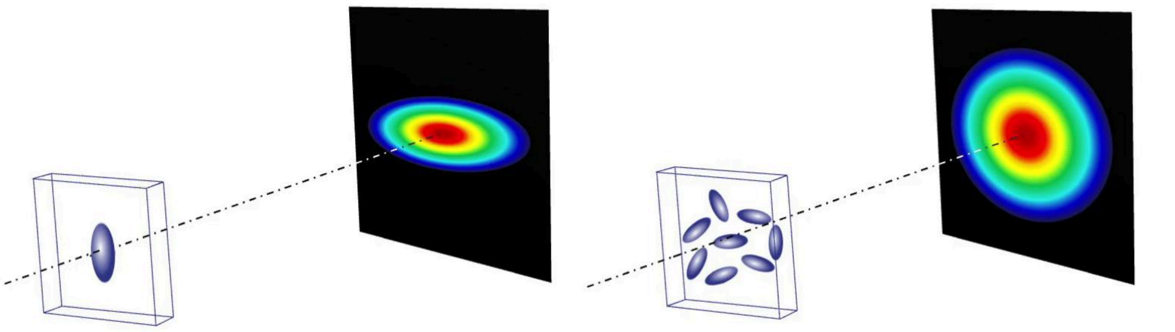
The scattering intensity is described by the equation shown here. Let's consider each term one at a time. In SAXS, we assume that the coherence volume is large enough that it can be coherently illuminated, but small enough for the concentration or number density of the particles being investigated that no two particles are illuminated within the same coherence volume. In this case, the intensity is proportional to the number density N. The scattering amplitude of a particle is proportional to both its volume and its electron density contrast with respect to any surrounding medium. The intensity is thus proportional to the square of these contributions. Likewise, the form factor FQ is directly proportional to the amplitude, and its square is thus proportional to the intensity. We've already stated that we are interested in those cases where the coherence volume doesn't contain more than one particle, hence, we can set this factor to unity. Lastly, we will also record contributions originating from background signal such as diffuse scattering from water. We need to subtract this. How this is done is explained in the next video. For the time being, we will ignore this, however.

Notes

Summary

2m 00s

# Scattering curves – single particle v random ensemble



Fixed orientation

Randomly oriented ensemble

$$I(\mathbf{Q})$$

$$I^{\mathrm{ro}}(Q) = \frac{n}{4\pi}\int_0^{2\pi} d\alpha \int_0^{\pi} \sin\beta \, d\beta \, I(\mathbf{Q})$$

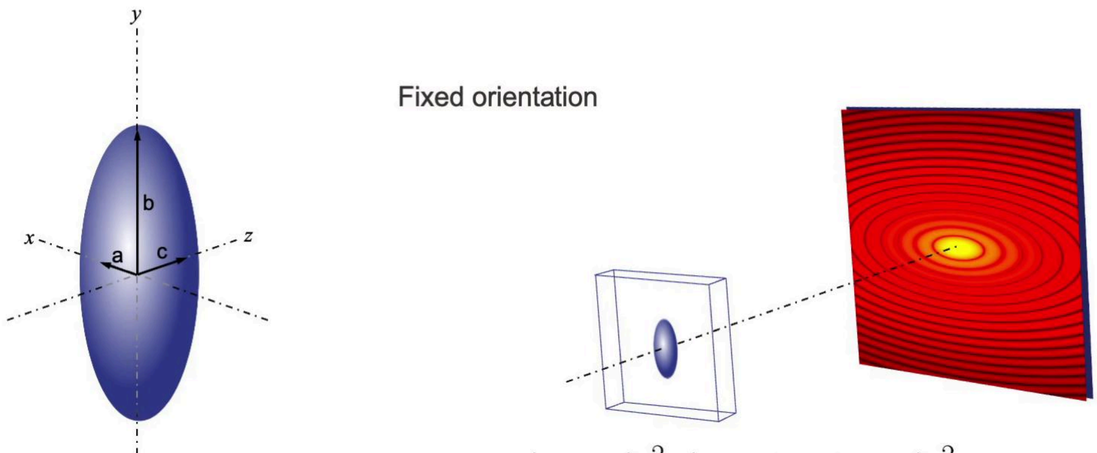
If a particle has a defined symmetry axis, in other words, if it is anything other than a sphere, then the SAXS pattern will depend on the orientation distribution of the ensemble of these particles. For an ensemble containing particles, all with the same fixed orientation, the SAXS pattern will be identical in form to that of a single particle. If, as is much more commonly the case, the particles are randomly oriented, one must integrate over all possible azimuthal and polar angles, given by alpha and beta respectively.

Notes

Summary

3m 25s

# Scattering curves – ellipsoid, fixed orientation




$$I_{\text{ell}}(\mathbf{Q}) = I_{\text{ell}}(Q_x, Q_y) = (r_0 \Delta\rho)^2 \left(\frac{4}{3}\pi abc\right)^2 \left(3\,\frac{\sin\phi - \phi\cos\phi}{\phi^3}\right)^2$$

$$\phi = \sqrt{a^2 Q_x^2 + b^2 Q_y^2}$$

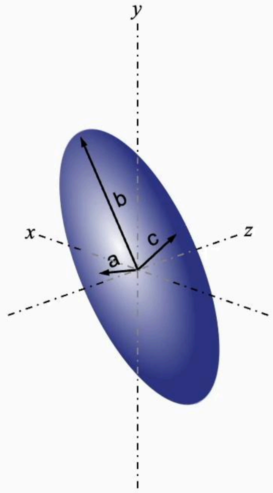
The scattering pattern of an ellipsoid, defined by semi-major and minor axes, A, B and C with the C axis pointing in the forward scattering direction is given by the expression shown here. The angle phi is defined as the hypotenuse of the product of the axes A and B, and their respective scattering vectors. Note that the more elongated the ellipse is in a given direction, the more compressed its scattering pattern in that same direction.

Notes

Summary

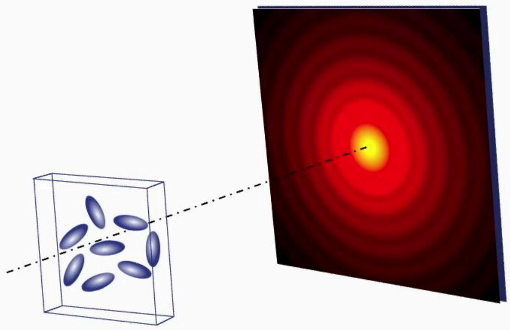
4m 04s

# Scattering curves – ellipsoid, randomly oriented ensemble




Average (integrate) over both polar angles α and β between 0 and $\pi/2$

Randomly oriented ensemble



$$I_{\text{ell}}^{\text{ro}}(Q) = (r_0 \Delta\rho)^2 \left(\frac{4}{3}\pi abc\right)^2$$
$$\times \frac{2}{\pi}\int_0^{\pi/2} d\alpha \int_0^{\pi/2} \sin\beta \, d\beta \left(3\,\frac{\sin\phi - \phi\cos\phi}{\phi^3}\right)^2$$

$$\phi = Q\sqrt{(a^2\sin^2\alpha + b^2\cos^2\alpha)\sin^2\beta + c^2\cos^2\beta}$$

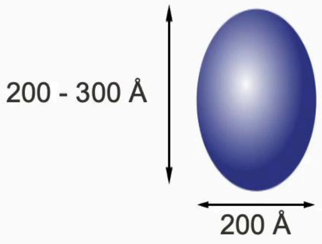
If the ensemble of ellipses is randomly oriented, we must again average over the azimuthal and polar angles as shown here. Now, if all the axes are equal in size, the ellipse becomes a sphere, and phi is equal to Qa, where there is no defined direction for Q as the pattern is as smoothly identical.

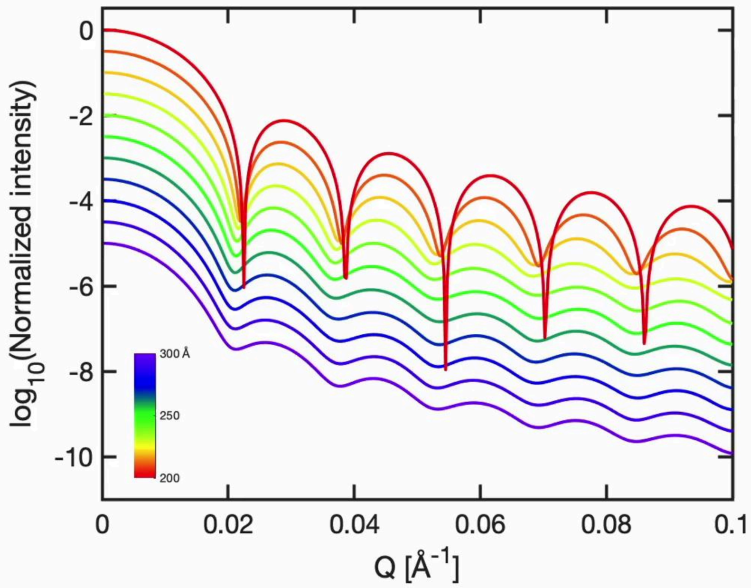
Notes

Summary

4m 37s

# Scattering curves – solid spheres



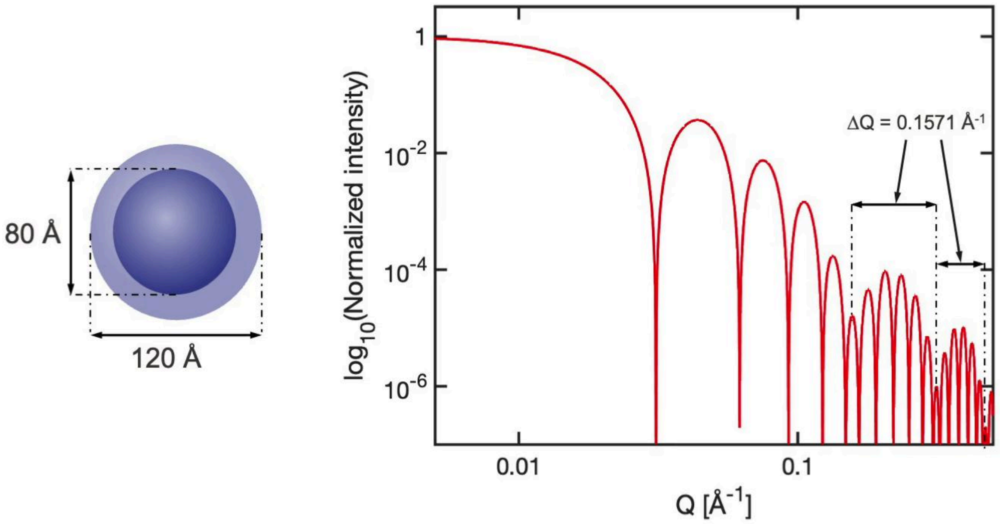

In this graph, we see the progress from a sphere to a randomly oriented set of ellipses, for which one axis is 50% larger than the other two. The interference fringes associated with the spheres become increasingly damped due to the orientational averaging.

Notes

Summary

5m 01s

# Scattering curves – hollow spheres




$$\Delta Q = 2\pi/(R_2 - R_1)$$

$$I(Q) = I_0 \left\{ \frac{3}{R_2^3 - R_1^3} \left[ \left( \frac{\sin(QR_2) - QR_2\cos(QR_2)}{Q^3} \right) - \left( \frac{\sin(QR_1) - QR_1\cos(QR_1)}{Q^3} \right) \right] \right\}^2$$

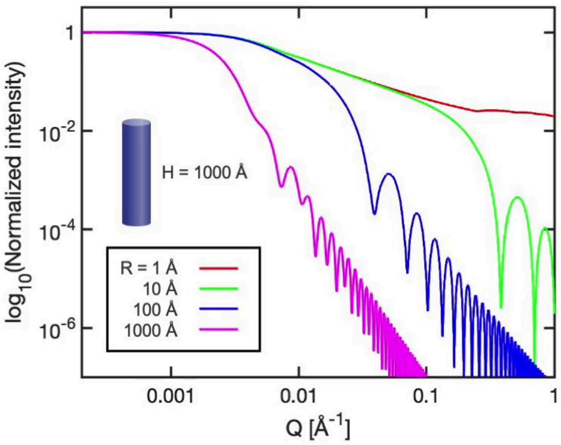
Hollow spheres are also very interesting models as they are often good approximations of cells with higher-density cell walls. Unsurprisingly, they have scattering patterns similar to solid spheres, but modulated by interference or beating between the patterns generated by scattering from the outer and inner surfaces. The modulation periodicity delta Q is equal to two pi divided by R2 minus R1 as shown here for a hollow shell with an outer and inner radius of 60 and 40 angstroms, respectively.

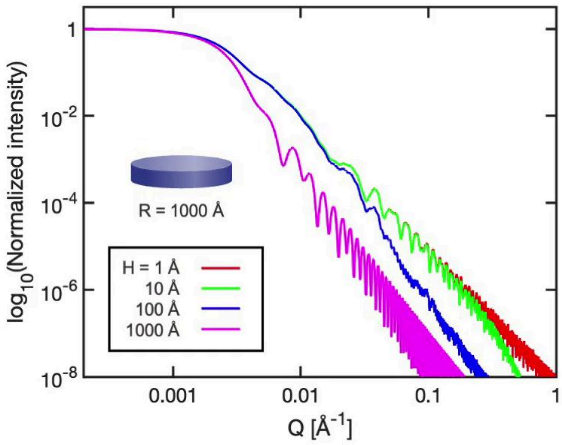
Notes

Summary

5m 20s

# Scattering curves – rods and platelets




$$I(Q) = 4\int_0^1 \frac{J_1^2[QR(1-x^2)^{1/2}]}{[QR(1-x^2)^{1/2}]^2} \cdot \frac{\sin^2(QHx/2)}{(QHx/2)^2}\, dx$$

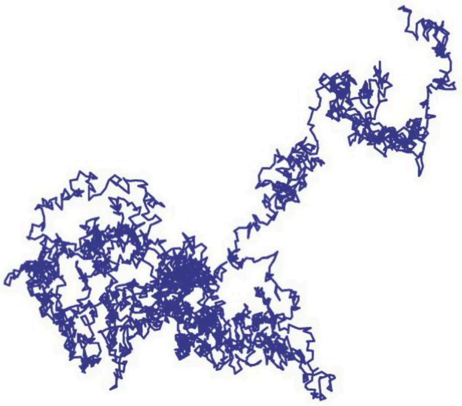
Rods and platelets are geometrically identified with a radius and height. They have scattering patterns for random orientations that are analytically defined by the frightening-looking equation provided here. J1 is the cylindrical Bessel function of the first kind, and integration is performed between the limits of X equals zero and one. The left-hand graph shows the progression of the pattern for rods from the radius being equal to the height to the radius being a thousand times smaller than the height. Conversely, on the right-hand side, the radius of a platelet is fixed at 1000 angstroms while the height is reduced to one angstrom. In both graphs, the rod curves are unrealistic as no object made of atoms can have a characteristic dimension as small as one angstrom.

Notes

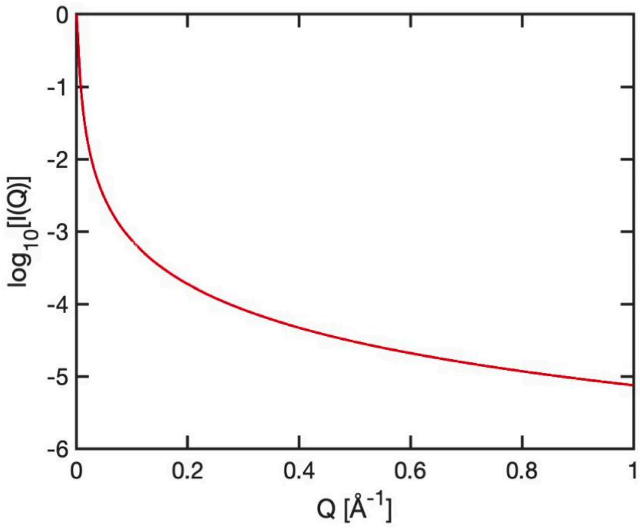
Summary

6m 00s

# Scattering curves – Gaussian chains



n links, each length a, random orientation
"Gaussian chain"




$$I(Q) = \frac{2I_0}{\phi^2}\left[\exp(-\phi) + \phi - 1\right] \quad \text{whereby} \quad \phi = Q^2 a^2 n/6$$

Lastly, so-called Gaussian chains are often good models to use for randomly folded polymeric strings such as denatured protein chains. The scattering pattern is given by the expression shown here where phi is equal to Q squared, a squared, n divided by six. where a is the link length, and n is the number of links in the chain.

Notes

Summary

6m 56s

# In the next video...

Now, in the next video, we complete our discussion of SAXS in general by looking at ways in which structural information can be extracted from different parts of the scattering curves, how a range of particle sizes impacts the SAXS signal, and lastly, a brief overview of some experimental considerations.

Notes

Summary

7m 21s