Today's Outline - March 03, 2015

Today's Outline - March 03, 2015

- SAXS review

Today's Outline - March 03, 2015

- SAXS review
- Calculating R_g

Today's Outline - March 03, 2015

- SAXS review
- Calculating R_g
- Porod regime

Today's Outline - March 03, 2015

- SAXS review
- Calculating R_g
- Porod regime
- Nucleation mechanism by SAXS

Today's Outline - March 03, 2015

- SAXS review
- Calculating R_g
- Porod regime
- Nucleation mechanism by SAXS

Homework Assignment #04:
Chapter 4: 2, 4, 6, 7, 10
due Monday, March 10, 2015

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$I^{SAXS}(\vec{Q}) = f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV_m$$

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$I^{SAXS}(\vec{Q}) = f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV_m$$

$$= f^2 \sum_n e^{i\vec{Q}\cdot\vec{r}_n} \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m$$

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$\begin{aligned}
I^{SAXS}(\vec{Q}) &= f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n-\vec{r}_m)} dV_m \\
&= f^2 \sum_n e^{i\vec{Q}\cdot\vec{r}_n} \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= f^2 \int_V \rho_{at} e^{i\vec{Q}\cdot\vec{r}_n} dV_n \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m
\end{aligned}$$

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$
\begin{aligned}
I^{SAXS}(\vec{Q}) &= f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV_m \\
&= f^2 \sum_n e^{i\vec{Q}\cdot\vec{r}_n} \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= f^2 \int_V \rho_{at} e^{i\vec{Q}\cdot\vec{r}_n} dV_n \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= \left| \int_V \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV \right|^2
\end{aligned}
$$

Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$
\begin{aligned}
I^{SAXS}(\vec{Q}) &= f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV_m \\
&= f^2 \sum_n e^{i\vec{Q}\cdot\vec{r}_n} \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= f^2 \int_V \rho_{at} e^{i\vec{Q}\cdot\vec{r}_n} dV_n \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= \left| \int_V \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV \right|^2
\end{aligned}
$$

Where we have assumed sufficient averaging and introduced $\rho_{sl} = f\rho_{at}$.

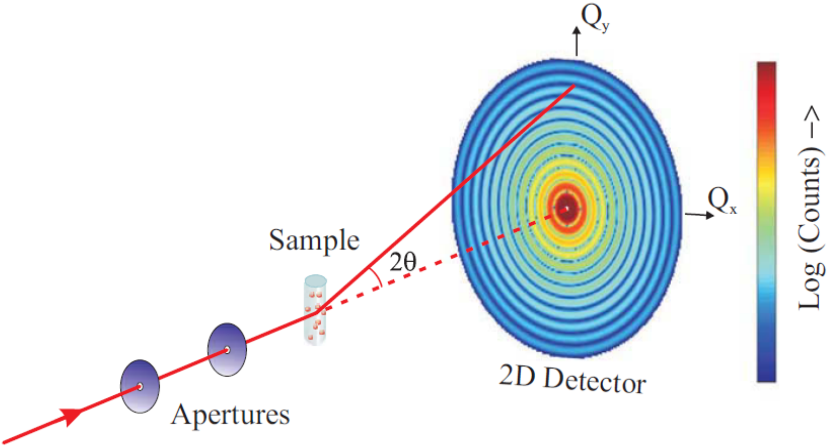
Small Angle Scattering

Recall that there was an additional term in the scattering intensity which becomes important at small Q.

$$
\begin{aligned}
I^{SAXS}(\vec{Q}) &= f^2 \sum_n \int_V \rho_{at} e^{i\vec{Q}\cdot(\vec{r}_n - \vec{r}_m)} dV_m \\
&= f^2 \sum_n e^{i\vec{Q}\cdot\vec{r}_n} \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= f^2 \int_V \rho_{at} e^{i\vec{Q}\cdot\vec{r}_n} dV_n \int_V \rho_{at} e^{-i\vec{Q}\cdot\vec{r}_m} dV_m \\
&= \left| \int_V \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV \right|^2
\end{aligned}
$$

Where we have assumed sufficient averaging and introduced $\rho_{sl} = f\rho_{at}$. This final expression looks just like an atomic form factor but the charge density that we consider here is on a much longer length scale than an atom.

The SAXS experiment



Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

Assume that the scattering length density of each identical particle (molecule) is given by $\rho_{sl,p}$ and the scattering length density of the solvent is $\rho_{sl,0}$.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

Assume that the scattering length density of each identical particle (molecule) is given by $\rho_{sl,p}$ and the scattering length density of the solvent is $\rho_{sl,0}$.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2 = (\rho_{sl,p} - \rho_{sl,0})^2 \left| \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

Assume that the scattering length density of each identical particle (molecule) is given by $\rho_{sl,p}$ and the scattering length density of the solvent is $\rho_{sl,0}$.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2 = (\rho_{sl,p} - \rho_{sl,0})^2 \left| \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

If we introduce the single-particle form factor $\mathcal{F}(\vec{Q})$:

Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

Assume that the scattering length density of each identical particle (molecule) is given by $\rho_{sl,p}$ and the scattering length density of the solvent is $\rho_{sl,0}$.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2 = (\rho_{sl,p} - \rho_{sl,0})^2 \left| \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

If we introduce the single-particle form factor $\mathcal{F}(\vec{Q})$:

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p$$

Scattering from a dilute solution

The simplest case is for a dilute solution of non-interacting molecules.

Assume that the scattering length density of each identical particle (molecule) is given by $\rho_{sl,p}$ and the scattering length density of the solvent is $\rho_{sl,0}$.

$$I^{SAXS}(\vec{Q}) = \left| \int_{V_p} \rho_{sl} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2 = (\rho_{sl,p} - \rho_{sl,0})^2 \left| \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p \right|^2$$

If we introduce the single-particle form factor $\mathcal{F}(\vec{Q})$:

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_{V_p} e^{i\vec{Q}\cdot\vec{r}} dV_p$$

$$I^{SAXS}(\vec{Q}) = \Delta\rho^2 V_p^2 |\mathcal{F}(\vec{Q})|^2$$

Where $\Delta\rho = (\rho_{sl,p} - \rho_{sl,0})$, and the form factor depends on the morphology of the particle (size and shape).

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p}\int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p}\int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 \, dr$$

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\begin{aligned} \mathcal{F}(\vec{Q}) &= \frac{1}{V_p} \int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 \, dr \\ &= 3 \left[\frac{\sin(QR) - QR\cos(QR)}{Q^3 R^3} \right] \end{aligned}$$

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\begin{aligned}
\mathcal{F}(\vec{Q}) &= \frac{1}{V_p} \int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 \, dr \\
&= 3 \left[\frac{\sin(QR) - QR\cos(QR)}{Q^3 R^3} \right] \\
&\equiv \frac{3J_1(QR)}{QR}
\end{aligned}$$

Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p}\int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\begin{aligned}
\mathcal{F}(\vec{Q}) &= \frac{1}{V_p}\int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 \, dr \\
&= 3\left[\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3}\right] \\
&\equiv \frac{3J_1(QR)}{QR}
\end{aligned}$$

Where $J_1(x)$ is the Bessel function of the first kind

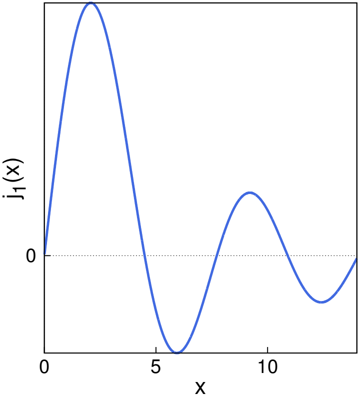
Scattering from a sphere

There are only a few morphologies which can be computed exactly and the simplest is a constant density sphere of radius R.

$$\mathcal{F}(\vec{Q}) = \frac{1}{V_p}\int_0^R \int_0^{2\pi} \int_0^{\pi} e^{iQr\cos\theta} r^2 \sin\theta \, d\theta \, d\phi \, dr$$

$$\begin{aligned}\mathcal{F}(\vec{Q}) &= \frac{1}{V_p}\int_0^R 4\pi \frac{\sin(Qr)}{Qr} r^2 \, dr \\ &= 3\left[\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3}\right] \\ &\equiv \frac{3J_1(QR)}{QR}\end{aligned}$$

Where $J_1(x)$ is the Bessel function of the first kind



Scattering from a sphere

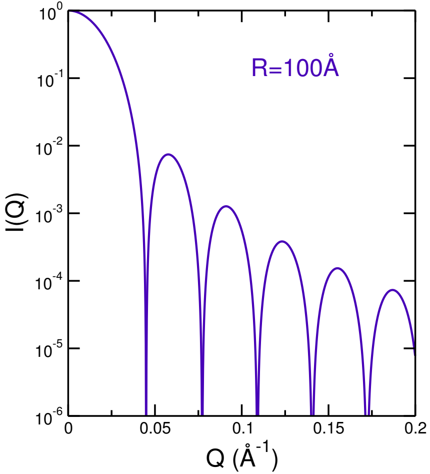
$$I(vectQ) = \Delta\rho^2 V_p^2 \left| \frac{3J_1(QR)}{QR} \right|^2$$

Scattering from a sphere

$$I(vectQ) = \Delta\rho^2 V_p^2 \left| \frac{3J_1(QR)}{QR} \right|^2 = \Delta\rho^2 V_p^2 \left| 3\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3} \right|^2$$

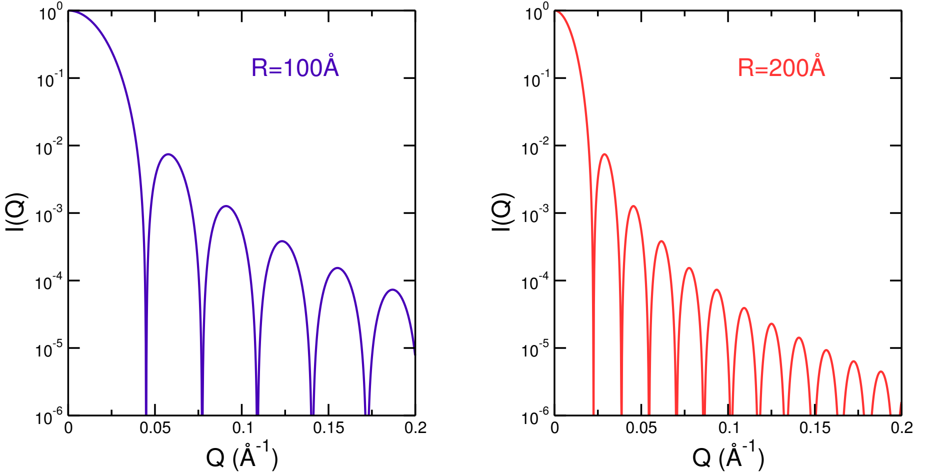
Scattering from a sphere

$$I(vectQ) = \Delta\rho^2 V_p^2 \left| \frac{3J_1(QR)}{QR} \right|^2 = \Delta\rho^2 V_p^2 \left| 3\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3} \right|^2$$



Scattering from a sphere

$$I(vectQ) = \Delta\rho^2 V_p^2 \left| \frac{3J_1(QR)}{QR} \right|^2 = \Delta\rho^2 V_p^2 \left| 3\frac{\sin(QR) - QR\cos(QR)}{Q^3R^3} \right|^2$$



Guinier analysis

In the long wavelength limit $QR \rightarrow 0$ we can approximate the scattering factor with the first terms of the sum

Guinier analysis

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots \right. \\ \left. - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

Guinier analysis

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots \right.$$
$$\left. - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

this simplifies to $\qquad \mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10} and$

Guinier analysis

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots \right.$$
$$\left. - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

this simplifies to $$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10} and$$

$$I^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 \left[1 - \frac{Q^2R^2}{10}\right]^2$$

Guinier analysis

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots \right.$$
$$\left. - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

this simplifies to $$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10} and$$

$$I^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 \left[1 - \frac{Q^2R^2}{10}\right]^2 \approx \Delta\rho^2 V_p^2 \left[1 - \frac{Q^2R^2}{5}\right]$$

Guinier analysis

In the long wavelength limit $QR \to 0$ we can approximate the scattering factor with the first terms of the sum

$$\mathcal{F}(Q) \approx \frac{3}{Q^3R^3}\left[QR - \frac{Q^3R^3}{6} + \frac{Q^5R^5}{120} - \cdots \right.$$
$$\left. - QR\left(1 - \frac{Q^2R^2}{2} + \frac{Q^4R^4}{24} - \cdots\right)\right]$$

this simplifies to $$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10} and$$

$$I^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 \left[1 - \frac{Q^2R^2}{10}\right]^2 \approx \Delta\rho^2 V_p^2 \left[1 - \frac{Q^2R^2}{5}\right]$$
$$\approx \Delta\rho^2 V_p^2 e^{-Q^2R^2/5}, \qquad QR \ll 1$$

Guinier analysis

In the long wavelength limit ($QR \to 0$), the form factor becomes

Guinier analysis

In the long wavelength limit ($QR \to 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2 R^2}{10}$$

Guinier analysis

In the long wavelength limit ($QR \to 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2 R^2}{10}$$
$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R^2/5}$$

Guinier analysis

In the long wavelength limit ($QR \rightarrow 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2 R^2}{10}$$
$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R^2/5}$$

and the initial slope of the $\log(I)$ vs Q^2 plot is $-R^2/5$

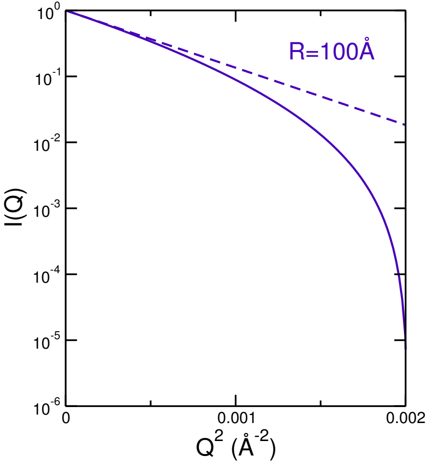
Guinier analysis

In the long wavelength limit ($QR \rightarrow 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2 R^2}{10}$$

$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R^2/5}$$

and the initial slope of the $\log(I)$ vs Q^2 plot is $-R^2/5$

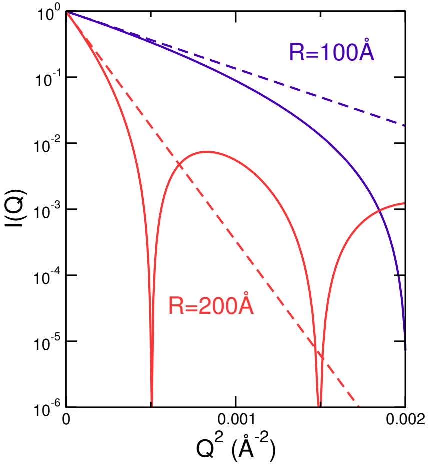


Guinier analysis

In the long wavelength limit ($QR \to 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10}$$
$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2R^2/5}$$

and the initial slope of the $\log(I)$ vs Q^2 plot is $-R^2/5$



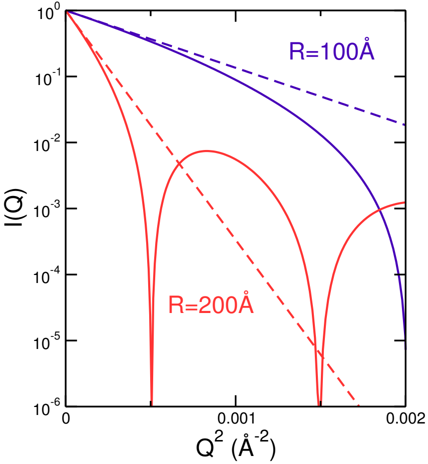
Guinier analysis

In the long wavelength limit ($QR \rightarrow 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10}$$
$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2R^2/5}$$

and the initial slope of the $\log(I)$ vs Q^2 plot is $-R^2/5$

In terms of the radius of gyration, R_g, which for a sphere is given by $\sqrt{\frac{3}{5}}R$



Guinier analysis

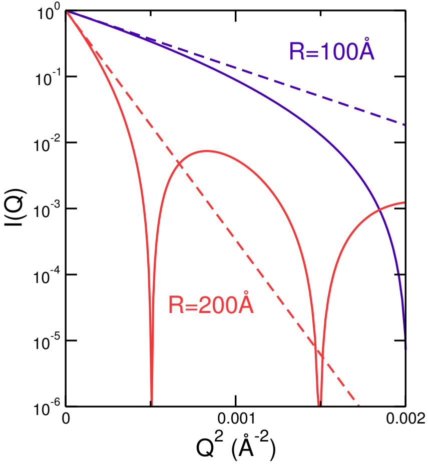
In the long wavelength limit ($QR \to 0$), the form factor becomes

$$\mathcal{F}(Q) \approx 1 - \frac{Q^2R^2}{10}$$
$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2R^2/5}$$

and the initial slope of the $\log(I)$ vs Q^2 plot is $-R^2/5$

In terms of the radius of gyration, R_g, which for a sphere is given by $\sqrt{\frac{3}{5}}R$

$$I(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2R_g^2/3}$$



Calculation of R_g

$$R_g^2 = \frac{1}{V_p} \int_{V_p} r^2 dV_p$$

Calculation of R_g

$$R_g^2 = \frac{1}{V_p}\int_{V_p} r^2 dV_p$$

In terms of the scattering length density, we have

Calculation of R_g

$$R_g^2 = \frac{1}{V_p}\int_{V_p} r^2 dV_p$$

$$= \frac{\int_{V_p} \rho_{sl,p}(\vec{r}) r^2 dV_p}{\int_{V_p} \rho_{sl,p}(\vec{r}) dV_p}$$

In terms of the scattering length density, we have

Calculation of R_g

$$R_g^2 = \frac{1}{V_p} \int_{V_p} r^2 dV_p = \frac{\int_{V_p} \rho_{sl,p}(\vec{r}) r^2 dV_p}{\int_{V_p} \rho_{sl,p}(\vec{r}) dV_p}$$

In terms of the scattering length density, we have

after orientational averaging this expression can be used to extract R_g from experimental data using

Calculation of R_g

$$R_g^2 = \frac{1}{V_p}\int_{V_p} r^2 dV_p$$
$$= \frac{\int_{V_p}\rho_{sl,p}(\vec{r})r^2 dV_p}{\int_{V_p}\rho_{sl,p}(\vec{r})dV_p}$$

In terms of the scattering length density, we have

after orientational averaging this expression can be used to extract R_g from experimental data using

$$I_1^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R_g^2/3}$$

Calculation of R_g

$$R_g^2 = \frac{1}{V_p}\int_{V_p} r^2 dV_p$$

$$= \frac{\int_{V_p} \rho_{sl,p}(\vec{r}) r^2 dV_p}{\int_{V_p} \rho_{sl,p}(\vec{r}) dV_p}$$

In terms of the scattering length density, we have

after orientational averaging this expression can be used to extract R_g from experimental data using

$$I_1^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R_g^2/3}$$

this expression holds for uniform and non-uniform densities

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$
$$\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right]$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$

$$\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right]$$

$$I(Q) = 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$
$$\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right]$$
$$I(Q) = 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2$$
$$= 9\Delta\rho^2 V_p^2 \frac{\left\langle \cos^2(QR)\right\rangle}{Q^4R^4}$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\begin{aligned}
\mathcal{F}(Q) &= 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right] \\
&\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right] \\
I(Q) &= 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2 \\
&= 9\Delta\rho^2 V_p^2 \frac{\left\langle\cos^2(QR)\right\rangle}{Q^4R^4} \\
&= \frac{9\Delta\rho^2 V_p^2}{Q^4R^4}\left(\frac{1}{2}\right)
\end{aligned}$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\begin{aligned}
\mathcal{F}(Q) &= 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right] \\
&\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right] \\
I(Q) &= 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2 \\
&= 9\Delta\rho^2 V_p^2 \frac{\langle\cos^2(QR)\rangle}{Q^4R^4} \\
&= \frac{9\Delta\rho^2 V_p^2}{Q^4R^4}\left(\frac{1}{2}\right) \\
I(Q) &= \frac{2\pi\Delta\rho^2}{Q^4} S_p
\end{aligned}$$

Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$

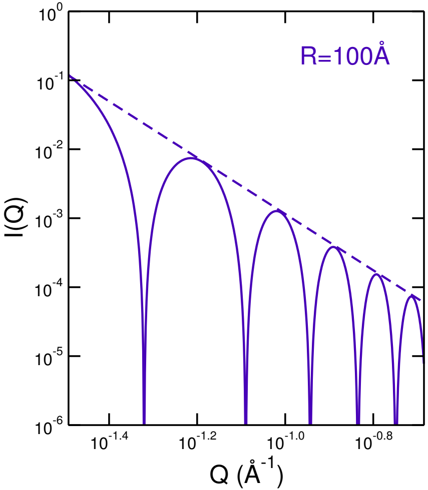
$$\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right]$$

$$I(Q) = 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2$$

$$= 9\Delta\rho^2 V_p^2 \frac{\langle\cos^2(QR)\rangle}{Q^4R^4}$$

$$= \frac{9\Delta\rho^2 V_p^2}{Q^4R^4}\left(\frac{1}{2}\right)$$

$$I(Q) = \frac{2\pi\Delta\rho^2}{Q^4} S_p$$



Porod analysis

In the short wavelength limit ($QR \gg 1$), the form factor for a sphere can be approximated

$$\mathcal{F}(Q) = 3\left[\frac{\sin(QR)}{Q^3R^3} - \frac{\cos(QR)}{Q^2R^2}\right]$$

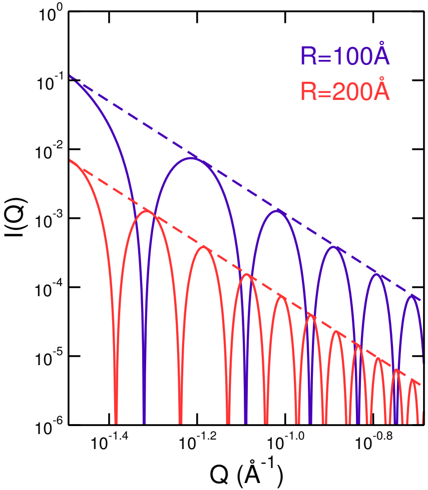
$$\approx 3\left[-\frac{\cos(QR)}{Q^2R^2}\right]$$

$$I(Q) = 9\Delta\rho^2 V_p^2 \left[-\frac{\cos(QR)}{Q^2R^2}\right]^2$$

$$= 9\Delta\rho^2 V_p^2 \frac{\langle\cos^2(QR)\rangle}{Q^4R^4}$$

$$= \frac{9\Delta\rho^2 V_p^2}{Q^4R^4}\left(\frac{1}{2}\right)$$

$$I(Q) = \frac{2\pi\Delta\rho^2}{Q^4} S_p$$



power law drop as Q^{-4} for spheres

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its "dimensionality" is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its "dimensionality" is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

$$dV_p = 4\pi r^2 dr \qquad \text{sphere}$$

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its “dimensionality” is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

$$dV_p = 4\pi r^2 dr \qquad \text{sphere}$$
$$dA_p = 2\pi r dr \qquad \text{disk}$$

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its "dimensionality" is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

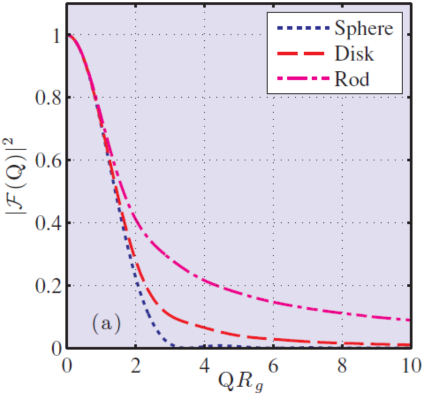
$$\begin{aligned} dV_p &= 4\pi r^2 dr && \text{sphere} \\ dA_p &= 2\pi r dr && \text{disk} \\ dL_p &= dr && \text{rod} \end{aligned}$$

Shape effect on scattering

The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its "dimensionality" is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

$$dV_p = 4\pi r^2 dr \qquad \text{sphere} \quad \alpha = 4$$
$$dA_p = 2\pi r dr \qquad \text{disk}$$
$$dL_p = dr \qquad \text{rod}$$

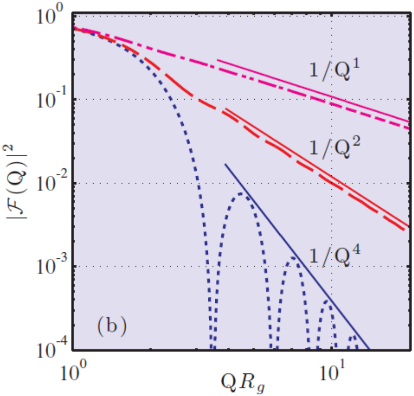


Shape effect on scattering

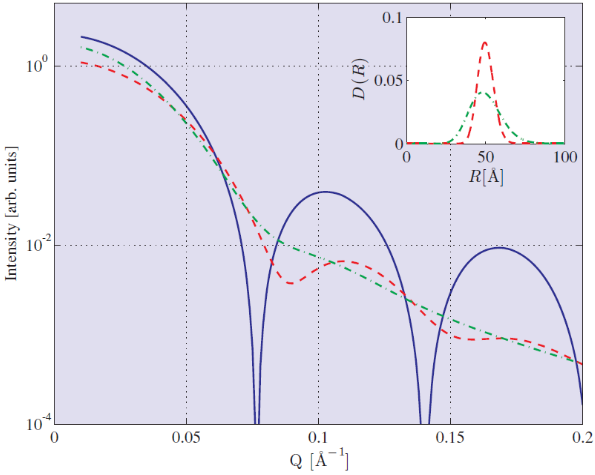
The shape of the particle will have a significant effect on the SAXS since the form factor is derived from an integral over the particle volume, V_p.

If the particle is not spherical, then its "dimensionality" is not 3 and this will affect the form factor and introduce a different power law in the Porod regime.

$$dV_p = 4\pi r^2 dr \qquad \text{sphere} \quad \alpha = 4$$
$$dA_p = 2\pi r dr \qquad \text{disk} \quad \alpha = 2$$
$$dL_p = dr \qquad \text{rod} \quad \alpha = 1$$

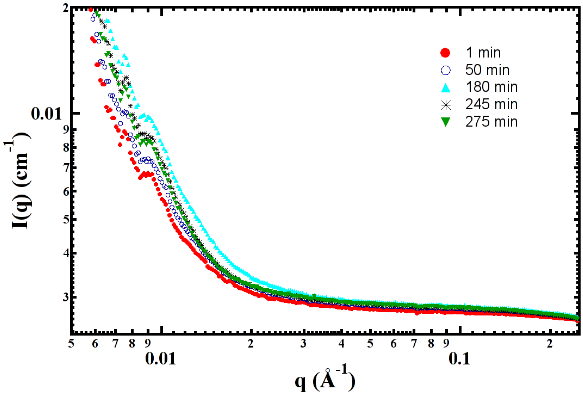


Polydispersivity



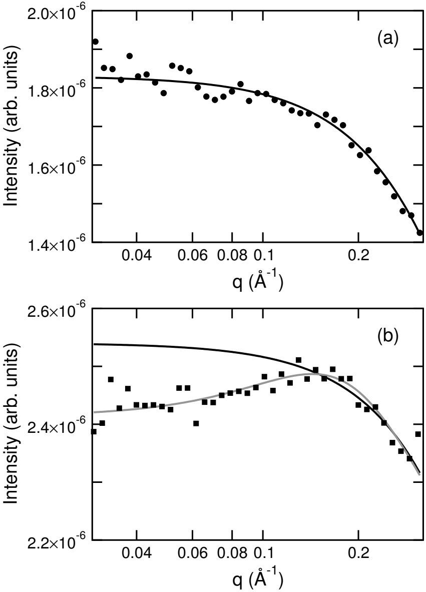
Nucleation & growth of glycine

Can SAXS help us understand the nucleation and growth of a simple molecule which is the prototype for pharmaceutical compounds?



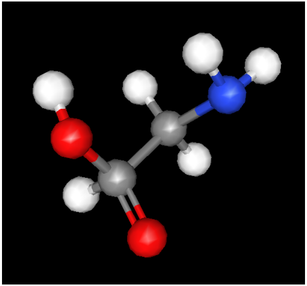
initial studies at 12 keV show change but no crystallization

Glycine nucleation

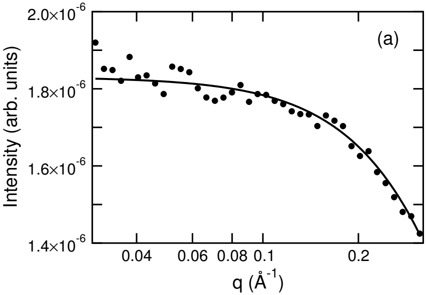


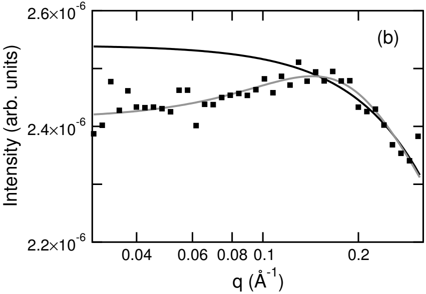
change to 25 keV x-rays

study neutral (top) and acidic (bottom) solutions



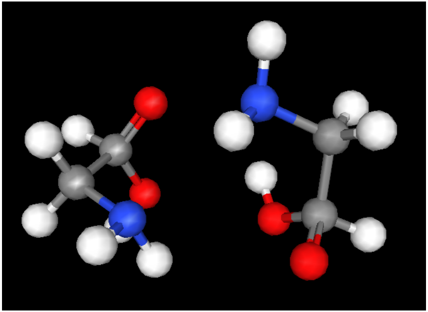
Glycine nucleation



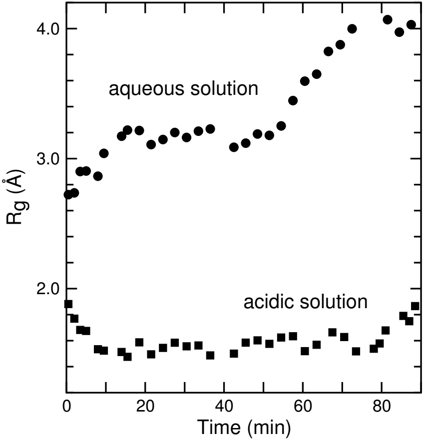


change to 25 keV x-rays

study neutral (top) and acidic (bottom) solutions



Glycine R_g



in aqueous solution, R_g implies dimerization and increases due to aggregation until crystallization

in acidic solution, Rg remains small and implies that no dimerization or aggregation occurs before nucleation

"Relationship between Self-Association of Glycine Molecules in Supersaturated Solution and Solid State Outcome", D. Erdemir et al. *Phys. Rev. Lett.* **99**, 115702 (2007)