Today’s Outline - February 20, 2018

• HW #02 solutions
• Liquid scattering
• Small angle x-ray scattering

Homework Assignment #03:
Chapter 3: 1, 3, 4, 6, 8
due Thursday, February 22, 2018
Today’s Outline - February 20, 2018

- HW #02 solutions
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- HW #02 solutions
- Liquid scattering
- Small angle x-ray scattering
- Calculating $R_g$
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• HW #02 solutions
• Liquid scattering
• Small angle x-ray scattering
• Calculating $R_g$

Homework Assignment #03:
Chapter 3:1,3,4,6,8
due Thursday, February 22, 2018
1. Knowing that the photoelectric absorption of an element scales as the inverse of the energy cubed, calculate:
   
   (a) the absorption coefficient at 10keV for copper when the value at 5keV is 1698.3 cm$^{-1}$;

   (b) The actual absorption coefficient of copper at 10keV is 1942.1 cm$^{-1}$, why is this so different than your calculated value?

2. A 30 cm long, ionization chamber, filled with 80% helium and 20% nitrogen gases at 1 atmosphere, is being used to measure the photon rate (photons/sec) in a synchrotron beamline at 12 keV. If a current of 10 nA is measured, what is the photon flux entering the ionization chamber?

3. A 5 cm deep ionization chamber is used to measure the fluorescence from a sample containing arsenic (As). Using any noble gases or nitrogen, determine a gas fill (at 1 atmosphere) for this chamber which absorbs at least 60% of the incident photons. How does this change if you are measuring the fluorescence from ruthenium (Ru)?
4. Calculate the critical angle of reflection of 10 keV and 30 keV x-rays for:

(a) A slab of glass (SiO₂);
(b) A thick chromium mirror;
(c) A thick platinum mirror.
(d) If the incident x-ray beam is 2 mm high, what length of mirror is required to reflect the entire beam for each material?

5. Calculate the fraction of silver (Ag) fluorescence x-rays which are absorbed in a 1 mm thick silicon (Si) detector and the charge pulse expected for each absorbed photon. Repeat the calculation for a 1 mm thick germanium (Ge) detector.
Knowing that the photoelectric absorption of an element scales as the inverse of the energy cubed, calculate

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(b) The actual absorption coefficient of copper at 10keV is 1942.1 cm\(^{-1}\), why is this so different than your calculated value?
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(a) We are given the energy dependence of the absorption coefficient and its value at 5keV.
Knowing that the photoelectric absorption of an element scales as the inverse of the energy cubed, calculate

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(a) We are given the energy dependence of the absorption coefficient and its value at 5keV. 
\[
\frac{\mu_{10\text{keV}}}{\mu_{5\text{keV}}} = \frac{1/10^3}{1/5^3}
\]
Homework 02 - Problem 1

Knowing that the photoelectric absorption of an element scales as the inverse of the energy cubed, calculate

(a) The absorption coefficient at 10keV for copper when the value at 5keV is $1698.3 \text{ cm}^{-1}$.

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\[
\frac{\mu_{10\text{keV}}}{\mu_{5\text{keV}}} = \frac{1/10^3}{1/5^3}
\]

\[
\mu_{10\text{keV}} = \mu_{5\text{keV}} \left(\frac{5}{10}\right)^3
\]
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\[
= 1698.3 \text{ cm}^{-1} \left(\frac{1}{8}\right)
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\[
= 1698.3 \text{ cm}^{-1} \left(\frac{1}{8}\right) = 212 \text{ cm}^{-1}
\]
Homework 02 - Problem 1

Knowing that the photoelectric absorption of an element scales as the inverse of the energy cubed, calculate

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(b) The actual absorption coefficient of copper at 10keV is 1942.1 cm$^{-1}$, why is this so different than your calculated value?

(a) We are given the energy dependence of the absorption coefficient and its value at 5 keV. \[
\frac{\mu_{10\text{keV}}}{\mu_{5\text{keV}}} = \frac{1/10^3}{1/5^3}
\]

(b) The calculation does not take into account the Cu K absorption edge at 8.98 keV.

\[
\mu_{10\text{keV}} = \mu_{5\text{keV}} \left(\frac{5}{10}\right)^3
\]

\[
= 1698.3 \text{ cm}^{-1} \left(\frac{1}{8}\right) = 212 \text{ cm}^{-1}
\]
Homework 02 - Problem 2

A 30 cm long, ionization chamber, filled with 80% helium and 20% nitrogen gases at 1 atmosphere, is being used to measure the photon rate (photons/sec) in a synchrotron beamline at 12 keV. If a current of \( i = 10 \text{ nA} \) is measured, what is the photon flux entering the ionization chamber?
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The number of free electrons per second generated in the ion chamber by the beam is given by

$$dN/dt = f(E) \Phi E W$$
A 30 cm long, ionization chamber, filled with 80% helium and 20% nitrogen gases at 1 atmosphere, is being used to measure the photon rate (photons/sec) in a synchrotron beamline at 12 keV. If a current of $i = 10 \text{nA}$ is measured, what is the photon flux entering the ionization chamber?

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where $f(E)$ is the fraction of the beam absorbed, $\Phi$ is the total flux incident on the ion chamber, $E$ is the energy of a single photon, and $W$ is the energy required to produce a free electron in the gas mixture.
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$$f(E) = \frac{l_0 - l(L)}{l_0}$$
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$$f(E) = \frac{l_0 - l(L)}{l_0} = 1 - e^{-\mu L}$$
The total absorption coefficient $\mu$ is a weighted sum of the absorption of the substance in the ion chamber.

\[
\mu = N \sum_{i=1}^{\infty} x_i \mu_i
\]

These values can be computed or looked up in the orange book or on the MuCal online calculator for the energy desired. For $E = 12$ keV, the photoelectric cross-section is $\mu = 2.0 \times 10^{-6} \text{ cm}^{-1}$. $\mu = 2.29 \times 10^{-3} \text{ cm}^{-1} \mu = 0.8 \mu$. $\mu = 0.2 \mu$. $\mu = 0.29 \times 10^{-3} \text{ cm}^{-1} \mu = 4.60 \times 10^{-4} \text{ cm}^{-1}$.
The total absorption coefficient $\mu$ is a weighted sum of the absorption of the substance in the ion chamber.

$$\mu = \sum_{i=1}^{N} x_i \mu_i$$
The total absorption coefficient $\mu$ is a weighted sum of the absorption of the substance in the ion chamber. Where the quantity $\mu_i$ can be computed from the absorption cross section of each component ($\sigma_{a,i}$), its mass density ($\rho_{m,i}$), molar mass ($M_i$), and Avogadro’s number ($N_A$).

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These values can be computed or looked up in the orange book or on the MuCal online calculator for the energy desired. For $E = 12$ keV, the photoelectric cross-section is

$$\mu_{He} = 2.0 \times 10^{-6} \text{ cm}^{-1}$$
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These values can be computed or looked up in the orange book or on the MuCal online calculator for the energy desired. For $E = 12$ keV, the photoelectric cross-section is

$$\mu_{He} = 2.0 \times 10^{-6} \text{ cm}^{-1}$$

$$\mu_{N_2} = 2.29 \times 10^{-3} \text{ cm}^{-1}$$

$$\mu = 0.8\mu_{He} + 0.2\mu_{N_2}$$
The total absorption coefficient $\mu$ is a weighted sum of the absorption of the substance in the ion chamber. Where the quantity $\mu_i$ can be computed from the absorption cross section of each component ($\sigma_{a,i}$), its mass density ($\rho_{m,i}$), molar mass ($M_i$), and Avogadro’s number ($N_A$).

$$\mu = \sum_{i=1}^{N} x_i \mu_i$$

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These values can be computed or looked up in the orange book or on the MuCal online calculator for the energy desired. For $E = 12$ keV, the photoelectric cross-section is

$$\mu_{\text{He}} = 2.0 \times 10^{-6} \ \text{cm}^{-1}$$

$$\mu_{\text{N}_2} = 2.29 \times 10^{-3} \ \text{cm}^{-1}$$

$$\mu = 0.8 \mu_{\text{He}} + 0.2 \mu_{\text{N}_2} = 0.8 \cdot 2.0 \times 10^{-6} + 0.2 \cdot 2.29 \times 10^{-3}$$
The total absorption coefficient $\mu$ is a weighted sum of the absorption of the substance in the ion chamber. Where the quantity $\mu_i$ can be computed from the absorption cross section of each component ($\sigma_{a,i}$), its mass density ($\rho_{m,i}$), molar mass ($M_i$), and Avogadro’s number ($N_A$).

$$\mu = \sum_{i=1}^{N} x_i \mu_i$$

$$\mu_i = \left( \frac{\rho_{m,i} N_A}{M_i} \right) \sigma_{a,i}$$

These values can be computed or looked up in the orange book or on the MuCal online calculator for the energy desired. For $E = 12$ keV, the photoelectric cross-section is $\mu_{N_2} = 2.29 \times 10^{-3} \text{ cm}^{-1}$

$$\mu = 0.8 \mu_{He} + 0.2 \mu_{N_2} = 0.8 \cdot 2.0 \times 10^{-6} + 0.2 \cdot 2.29 \times 10^{-3}$$

$$= 4.60 \times 10^{-4} \text{ cm}^{-1}$$
Now we use this to calculate the fraction of photons absorbed in the chamber

\[ \frac{dN}{dt} = i_e = 10 \times 10^{-9} \times 6.02 \times 10^{-19} = 6.24 \times 10^{10} \text{ s}^{-1} \]

Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]

The number of electrons per second can be computed directly from the measured current

\[ W_{\text{He}} = 41 \text{ eV} \]
\[ W_{\text{N}_2} = 36 \text{ eV} \]
\[ W_{\text{He}} = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV} \]

Putting it all together

\[ \Phi = \frac{dN}{dt} W_f(E_E) E = (6.24 \times 10^{10}) (40 \text{ eV}) (0.0136) (12 \times 10^3 \text{ eV/photon}) = 1.53 \times 10^{10} \text{ photon/s} \]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[ f(E) = 1 - e^{-\mu L} \]

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[ f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \times 30} \]

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]

The number of electrons per second can be computed directly from the measured current:

\[ \Phi = \frac{dN}{dt} \frac{W}{f(E)} \]

Putting it all together:

\[ \Phi = \frac{dN}{dt} \frac{W}{f(E)} = \frac{6.24 \times 10^{-10}}{6.0136 \times 10^3} \text{ photons/s} \]

\[ = 1.53 \times 10^{10} \text{ photons/s} \]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]

\[ f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30} \]

\[ = 0.0136 = 1.36\% \]
Now we use this to calculate the fraction of photons absorbed in the chamber.

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]

\[ f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \times 30} \]

\[ = 0.0136 = 1.36\% \]

The number of electrons per second can be computed directly from the measured current.
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e}
\]

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 4.30}
\]

\[
= 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}}
\]

\[\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}\]

\[f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30}\]

\[= 0.0136 = 1.36\%\]

The number of electrons per second can be computed directly from the measured current
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
\]

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4}}\cdot 30 = 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current
Homework 02 - Problem 2 (cont.)

Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
\]

Finally, we look up in the orange book the energy required to make a free electron by inoization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 4.30}
\]

\[
= 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
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Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
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\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30} = 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
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Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30} = 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]

\[
W = 0.8 \cdot 41 + 0.2 \cdot 36
\]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
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Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30} = 0.0136 = 1.36\%
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The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]

\[
W = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV}
\]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
\]

Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
\]

\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 4.30^{-4}} = 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]

\[
W = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV}
\]

Putting it all together
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
\]

Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
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\[
f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 4.30} = 0.0136 = 1.36\%
\]

The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]

\[
W = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV}
\]

Putting it all together

\[
\Phi = \frac{dN}{dt} \frac{W}{f(E)E}
\]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[
\frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1}
\]

Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[
\mu = 4.60 \times 10^{-4} \text{ cm}^{-1}
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f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 10^{-4} \cdot 30} = 0.0136 = 1.36\%
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The number of electrons per second can be computed directly from the measured current

\[
W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV}
\]

\[
W = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV}
\]

Putting it all together

\[
\Phi = \frac{dN}{dt} \frac{W}{f(E)E} = \frac{(6.24 \times 10^{10} \text{ s}^{-1})(40 \text{ eV})}{(0.0136)(12 \times 10^3 \text{ eV/photon})}
\]
Now we use this to calculate the fraction of photons absorbed in the chamber

\[ \frac{dN}{dt} = \frac{i}{e} = \frac{10 \times 10^{-9}}{1.602 \times 10^{-19}} = 6.24 \times 10^{10} \text{ s}^{-1} \]

Finally, we look up in the orange book the energy required to make a free electron by ionization for each gas and take a weighted average

\[ \mu = 4.60 \times 10^{-4} \text{ cm}^{-1} \]

\[ f(E) = 1 - e^{-\mu L} = 1 - e^{-4.60 \times 4.30} = 0.0136 = 1.36\% \]

The number of electrons per second can be computed directly from the measured current

\[ W_{He} = 41 \text{ eV} \quad W_{N_2} = 36 \text{ eV} \]

\[ W = 0.8 \cdot 41 + 0.2 \cdot 36 = 40 \text{ eV} \]

Putting it all together

\[ \Phi = \frac{dN}{dt} \frac{W}{f(E)E} = \frac{(6.24 \times 10^{10} \text{ s}^{-1})(40 \text{ eV})}{(0.0136)(12 \times 10^3 \text{ eV/photon})} = 1.53 \times 10^{10} \text{ photon/s} \]
A 5 cm deep ionization chamber is used to measure the fluorescence from a sample containing arsenic (As). Using any noble gases or nitrogen, determine a gas fill (at 1 atmosphere) for this chamber which absorbs at least 60% of the incident photons. How does this change if you are measuring the fluorescence from ruthenium (Ru)?
A 5 cm deep ionization chamber is used to measure the fluorescence from a sample containing arsenic (As). Using any noble gases or nitrogen, determine a gas fill (at 1 atmosphere) for this chamber which absorbs at least 60% of the incident photons. How does this change if you are measuring the fluorescence from ruthenium (Ru)?

The energy of the arsenic fluorescence line can be obtained from MuCal or from Hephaestus and is 10.54 keV. We would like to have at least 60% absorption in the 5 cm chamber. This can give us the desired value of $\mu$.
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Homework 02 - Problem 3

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This is the minimum value of the absorption that we require.

\[
f(E) = 1 - e^{-\mu L}
\]

\[
e^{-\mu L} = [1 - f(E)]
\]

\[
-\mu L = \ln[1 - f(E)]
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Thus for the most likely candidates we have:

- $f(E)_{Kr} = 1 - e^{-0.17 \times 5} = 1 - 0.43 = 57\%$
- $f(E)_{Xe} = 1 - e^{-0.89 \times 5} = 1 - 0.01 = 99\%$

For the Ru K-edge at 19.28 keV, we have:

- $\mu_{Ar} = 0.017 \text{ cm}^{-1}$
- $\mu_{Kr} = 0.23 \text{ cm}^{-1}$
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Homework 02 - Problem 3 (cont.)

Looking at tabulated values of the absorption coefficient for various gases at this energy (from MuCal, *total* cross-section):

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\[ f(E)_{\text{Xe}} = 1 - e^{- (0.89)(5)} = 1 - 0.01 = 99\% \]

For the Ru K-edge at 19.28 keV, we have

\[ \mu_{\text{Ar}} = 0.017 \text{ cm}^{-1} \quad \mu_{\text{Kr}} = 0.23 \text{ cm}^{-1} \quad \mu_{\text{Xe}} = 0.17 \text{ cm}^{-1} \quad \mu_{\text{Rn}} = 0.99 \text{ cm}^{-1} \]

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\[ f(E)_{\text{Xe}} = 1 - e^{- (0.17)(5)} = 1 - 0.43 = 57\% \]
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Looking at tabulated values of the absorption coefficient for various gases at this energy (from MuCal, total cross-section):

\[ \mu_{He} = 4.2 \times 10^{-5} \text{ cm}^{-1} \quad \mu_{N_2} = 3.9 \times 10^{-3} \text{ cm}^{-1} \quad \mu_{Ne} = 8.8 \times 10^{-3} \text{ cm}^{-1} \]
\[ \mu_{Ar} = 0.098 \text{ cm}^{-1} \quad \mu_{Kr} = 0.17 \text{ cm}^{-1} \quad \mu_{Xe} = 0.89 \text{ cm}^{-1} \quad \mu_{Rn} = 1.3 \text{ cm}^{-1} \]

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Homework 02 - Problem 4

Calculate the characteristic angle of reflection of 10keV and 30keV x-rays for:

(a) A slab of glass (SiO$_2$)
(b) A thick chromium mirror;
(c) A thick platinum mirror.
(d) If the incident x-ray beam is 2mm high, what length of mirror is required to reflect the entire beam for each material?
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The critical angle is related to the index of refraction, with

\[ \alpha_c = \sqrt{2\delta}, \quad \delta = \frac{2\pi \rho r_0}{k^2} \]

\[ r_0 = 2.82 \times 10^{-5} \text{Å} \]
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The critical angle is related to the index of refraction, with
\[ r_0 = 2.82 \times 10^{-5} \text{Å} \]

the electron density \( \rho \) can be computed using the mass density, \( \rho_m \)

\[ \rho[\text{e}^-/\text{Å}^3] = \frac{\rho_m[\text{g/cm}^3] \cdot N_A[\text{atom/mol}] \cdot Z[\text{e}^-/\text{atom}]}{M[\text{g/mol}] \cdot (10^8[\text{Å/cm}])^3} \]
Homework 02 - Problem 4 (cont.)

The wave number for the radiation is given by

\[ k [\text{Å}^{-1}] = \frac{2\pi}{E [\text{keV}] \times 10^3} \times \left( 4.135 \times 10^{-15} \text{eV} \cdot \text{s} \right) \left( 3 \times 10^{18} \text{Å/s} \right) = 0.51 E [\text{keV}] \]

For the two energies specified (10 keV and 30 keV), we have

\[ \alpha_c = 3.71 \times 10^{-3} \sqrt{\rho} \]
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now the expression for the critical angle becomes

\[ \alpha_c = \sqrt{\frac{4\pi(2.82 \times 10^{-5}[\text{Å}])(\sqrt[3]{\rho[\text{e}^-/\text{Å}^3]/k[\text{Å}^{-1}]}^2}}{k[\text{Å}^{-1}]} \]
The wave number for the radiation is given by

\[
k\left[\text{Å}^{-1}\right] = \frac{2\pi E}{hc} = \frac{2\pi E [\text{keV}] \times 10^3}{(4.135 \times 10^{-15} \text{[eV} \cdot \text{s]})) (3 \times 10^{18} \text{[Å/s]})} = 0.51 E [\text{keV}]
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\alpha_c = \sqrt{4\pi (2.82 \times 10^{-5} \text{[Å]})} \sqrt{\frac{\rho [\text{e}^-/\text{Å}^3]}{k \text{[Å}^{-1}]}} = 3.71 \times 10^{-2} \sqrt{\frac{\rho [\text{e}^-/\text{Å}^3]}{E [\text{keV}]}}
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\[ \alpha_c = \sqrt{4\pi (2.82 \times 10^{-5} [\text{Å}])} \frac{\sqrt{\rho [\text{e}^{-} / \text{Å}^3]}}{k [\text{Å}^{-1}]} = 3.71 \times 10^{-2} \frac{\sqrt{\rho [\text{e}^{-} / \text{Å}^3]}}{E [\text{keV}]} \]

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\[ \alpha_{c10} = 3.71 \times 10^{-3} \sqrt{\rho}, \]
The wave number for the radiation is given by

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now the expression for the critical angle becomes

\[ \alpha_c = \sqrt{4\pi(2.82 \times 10^{-5}[Å])} \sqrt{\frac{\rho[\text{e}^-/Å^3]}{k[Å^{-1}]}} = 3.71 \times 10^{-2} \sqrt{\frac{\rho[\text{e}^-/Å^3]}{E[\text{keV}]}} \]

for the two energies specified (10 keV and 30 keV), we have

\[ \alpha_{c10} = 3.71 \times 10^{-3} \sqrt{\rho}, \quad \alpha_{c30} = 1.20 \times 10^{-3} \sqrt{\rho} \]
(a) for SiO₂, \( \rho_m = 2.2 \text{ g/cm}^2 \), \( M = 60 \text{ g/mol} \), \( Z = 30 \)
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$\rho = 0.662 \text{Å}^{-3}$, \hspace{1cm} $\alpha_{c10} = 3.02 \text{mrad} = 0.17^\circ$,
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\[\rho = 0.662\text{Å}^{-3}, \quad \alpha_{c10} = 3.02\text{mrad} = 0.17^\circ, \quad \alpha_{c30} = 1.01\text{mrad} = 0.06^\circ,\]
Homework 02 - Problem 4 (cont.)

(a) for SiO$_2$, $\rho_m = 2.2 \text{ g/cm}^2$, $M = 60 \text{ g/mol}$, $Z = 30$

$\rho = 0.662 \text{Å}^{-3}$, $\alpha_{c10} = 3.02 \text{mrad} = 0.17^\circ$, $\alpha_{c30} = 1.01 \text{mrad} = 0.06^\circ$,

(b) for Cr, $\rho_m = 7.19 \text{ g/cm}^2$, $M = 52 \text{ g/mol}$, $Z = 24$
Homework 02 - Problem 4 (cont.)

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(d) The length of the mirror required to capture the entire 2 mm high beam is given by

$L = 2 \text{mm}$ for the 6 cases in (a-c) we have

SiO$_2$ 0.67 m, 2.00 m
Cr 0.38 m, 1.14 m
Pt 0.25 m, 0.72 m
Homework 02 - Problem 4 (cont.)

(a) for SiO$_2$, $\rho_m = 2.2 \text{ g/cm}^2$, $M = 60 \text{ g/mol}$, $Z = 30$

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Homework 02 - Problem 4 (cont.)

(a) for SiO$_2$, $\rho_m = 2.2$ g/cm$^2$, $M = 60$ g/mol, $Z = 30$

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(c) for Pt, $\rho_m = 21.4$ g/cm$^2$, $M = 195$ g/mol, $Z = 78$

$\rho = 5.16\,\text{Å}^{-3}$, $\alpha_{c10} = 8.44\,\text{mrad} = 0.48^\circ$, 
Homework 02 - Problem 4 (cont.)

(a) for SiO$_2$, $\rho_m = 2.2$ g/cm$^2$, $M = 60$ g/mol, $Z = 30$

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(d) The length of the mirror required to capture the entire 2 mm high beam is given by

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- for Cr: $L = 0.38$ m
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At 10 keV and 30 keV.

C. Segre (IIT)
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<table>
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Homework 02 - Problem 5

Calculate the fraction of silver (Ag) fluorescence x-rays which are absorbed in a 1 mm thick silicon (Si) detector and the charge pulse expected for each absorbed photon. Repeat the calculation for a 1 mm thick germanium (Ge) detector.

The Ag K$_\alpha$ fluorescence line is at 22.2 keV and the absorption coefficients for Si and Ge at that energy are

$\mu_{\text{Si}} = 7.5 \text{ cm}^{-1}$,

$\mu_{\text{Ge}} = 168 \text{ cm}^{-1}$,

the percentage of photons absorbed is given by

$f(E) = \frac{I_0 - I(L)}{I_0} = 1 - e^{-\mu L}$

$f_{\text{Si}}(E) = 1 - e^{-(7.5 \times 0.1)} = 0.53 = 53\%$

$f_{\text{Ge}}(E) = 1 - e^{-(168 \times 0.1)} = 0.99 = 99\%$
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Calculate the fraction of silver (Ag) fluorescence x-rays which are absorbed in a 1 mm thick silicon (Si) detector and the charge pulse expected for each absorbed photon. Repeat the calculation for a 1 mm thick germanium (Ge) detector.

The Ag K$_\alpha$ fluorescence line is at 22.2 keV and the absorption coefficients for Si and Ge at that energy, are

$$\mu_{Si} = 7.5\text{cm}^{-1}, \quad \mu_{Ge} = 168\text{cm}^{-1},$$

the percentage of photons absorbed is given by

$$f(E) = \frac{l_0 - l(L)}{l_0} = 1 - e^{-\mu L}$$

$$f_{Si}(E) = 1 - e^{-(7.5)(0.1)} = 0.53 = 53\%$$

$$f_{Ge}(E) = 1 - e^{-(168)(0.1)} = 0.99 = 99\%,$$
The energy required to create an electron-hole pair ($W$) is 3.7 eV for Si and 3.0 eV for Ge, so the number of electrons produced is

$$N_{Si} = f_{Si}(E_{W}) = 0.53 \times 3.7 \times 10^4 = 3175$$

$$N_{Ge} = f_{Ge}(E_{W}) = 0.99 \times 3.0 \times 10^4 = 7393$$

We get the charge pulse by multiplying the charge per electron

$$\delta q_{Si} = 5.1 \times 10^{-16} C$$

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Liquid scattering review

The liquid scattering experiment measured the liquid structure factor, $S(Q)$, a short range order quantity.
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$$g(r) = 1 + \frac{1}{2\pi^2 r \rho_{at}} \int_0^\infty Q [S(Q) - 1] \sin(Qr) dQ$$

This formalism holds for both non-crystalline solids and liquids, even though inelastic scattering dominates in the latter.

The relation between radial distribution function and structure factor can be extended to multi-component systems where $g(r) \rightarrow g_{ij}(r)$ and $S(Q) \rightarrow S_{ij}(Q)$. 
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$$g(r, t) - 1 = \frac{1}{2\rho\pi^2r} \int \int e^{i\omega t} \sin(Qr)QS(Q, E) dQ dE$$

Water dynamics

The peak below 1.5 Å represents the self motion of the central atom while the data at longer distances represents the collective motions of two different atoms, in this case the oxygens. The first and second peaks are highly coupled in space and time and merge within 0.8 ps. This behavior is different from liquid metals and leads to the viscosity of water.

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Small angle x-ray scattering

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

\[ I(\mathbf{Q}) = f^2 \sum_n \int_V \rho_{at} e^{i \mathbf{Q} \cdot (\mathbf{r}_n - \mathbf{r}_m)} dV_m = f^2 \sum_n e^{i \mathbf{Q} \cdot \mathbf{r}_n} \int_V \rho_{at} e^{-i \mathbf{Q} \cdot \mathbf{r}_m} dV_m = f^2 \int_V \rho_{sl} e^{i \mathbf{Q} \cdot \mathbf{r}} dV \]

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.
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The SAXS experiment
Scattering from a dilute solution

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

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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 $R$. 

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

\[ F(Q) = \frac{1}{V_p} \int_0^R 4\pi \sin(Qr) Qr r^2 dr = 3 \left[ \sin(QR) - QR \cos(QR) \right] Q^3 R^3 \equiv 3 J_1(QR) QR \]

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

[Graph of $j_1(x)$]
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Guinier analysis

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

\[
F(Q) \approx 3Q^3R^3 - QR(1 - Q^2R^2/10 + \cdots)
\]

this simplifies to

\[
F(Q) \approx 1 - Q^2R^2/10
\]

and

\[
I_{SAXS}(Q) \approx \Delta \rho^2 V^2 p \left[ 1 - Q^2R^2/5 \right] \approx \Delta \rho^2 V^2 p e^{-Q^2R^2/5}, \quad QR \ll 1
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$$\mathcal{F}(Q) \approx \frac{3}{Q^3 R^3} \left[ QR - \frac{Q^3 R^3}{6} + \frac{Q^5 R^5}{120} - \cdots ight]$$

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

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

this simplifies to

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

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

$$\approx \Delta \rho^2 V_p^2 e^{-Q^2 R^2/5}, \quad QR \ll 1$$
Guinier analysis

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

\[
F(Q) \approx 1 - \frac{Q^2 R^2}{10} I(Q) \approx \Delta \rho^2 V^2 p - \frac{Q^2 R^2}{5}.
\]

In terms of the radius of gyration, \(R_g\), which for a sphere is given by

\[
\sqrt{\frac{3}{5}} R \approx \Delta \rho^2 V^2 p - \frac{Q^2 R_g^2}{3}.
\]
Guinier analysis

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I(Q) \approx \Delta \rho^2 V^2_p e^{-Q^2 R^2 / 5}
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and the initial slope of the \(\log(I)\) vs \(Q^2\) plot is \(-R^2/5\)
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Calculation of $R_g$

\[ R_g^2 = \frac{1}{V_p} \int_{V_p} r^2 \, dV_p \]
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Calculation of $R_g$

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Calculation of $R_g$

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\[ I_{1}^{SAXS}(Q) \approx \Delta \rho^2 V_p^2 e^{-Q^2 R_g^2/3} \]
Calculation of $R_g$

\[\begin{align*}
R_g^2 &= \frac{1}{V_p} \int_{V_p} r^2 \, dV_p \\
&= \frac{\int_{V_p} \rho_{sl,p}(\vec{r}) r^2 \, dV_p}{\int_{V_p} \rho_{sl,p}(\vec{r}) \, dV_p}
\end{align*}\]

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