Today's outline - August 26, 2021

Today's outline - August 26, 2021

- Molecule and crystal scattering factors

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice
- Compton (inelastic) scattering

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice
- Compton (inelastic) scattering
- X-ray absorption

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice
- Compton (inelastic) scattering
- X-ray absorption

Reading Assignment: Chapter 2.1–2.2

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice
- Compton (inelastic) scattering
- X-ray absorption

Reading Assignment: Chapter 2.1–2.2

Homework Assignment #01:
Chapter 2: 2,3,5,6,8
due Tuesday, September 07, 2021

Today's outline - August 26, 2021

- Molecule and crystal scattering factors
- Crystal lattice types
- The reciprocal lattice
- Compton (inelastic) scattering
- X-ray absorption

Reading Assignment: Chapter 2.1–2.2

Homework Assignment #01:
Chapter 2: 2,3,5,6,8
due Tuesday, September 07, 2021

Homework Assignment #02:
Problems on Blackboard
due Tuesday, September 21, 2021

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

Thomson scattering from a single electron $-r_0 = -\dfrac{e^2}{4\pi\epsilon_0 mc^2}$

$-r_0$ $= -r_0$

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

Thomson scattering from a single electron $-r_0 = -\dfrac{e^2}{4\pi\epsilon_0 mc^2}$

atomic form factor $f^0(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r$

$-r_0 f(\mathbf{Q}, \hbar\omega) = -r_0 \left[f^0(\mathbf{Q}) \right]$

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

Thomson scattering from a single electron	$-r_0 = -\dfrac{e^2}{4\pi\epsilon_0 mc^2}$
atomic form factor	$f^0(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r$
anomalous scattering terms	$f'(\hbar\omega) + if''(\hbar\omega)$

$$-r_0 f(\mathbf{Q}, \hbar\omega) = -r_0 \left[f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega) \right]$$

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

Thomson scattering from a single electron $-r_0 = -\dfrac{e^2}{4\pi\epsilon_0 mc^2}$

atomic form factor $f^0(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r$

anomalous scattering terms $f'(\hbar\omega) + if''(\hbar\omega)$

polarization factor $P = \begin{cases} 1 \\ \sin^2\Psi \\ \frac{1}{2}(1+\sin^2\Psi) \end{cases}$

$$-r_0 f(\mathbf{Q},\hbar\omega)\sin^2\Psi = -r_0\left[f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)\right]\sin^2\Psi$$

Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

From the *International Tables for Crystallography*

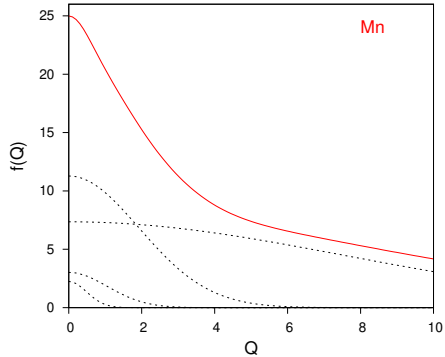
Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

From the *International Tables for Crystallography*



	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Mn	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896

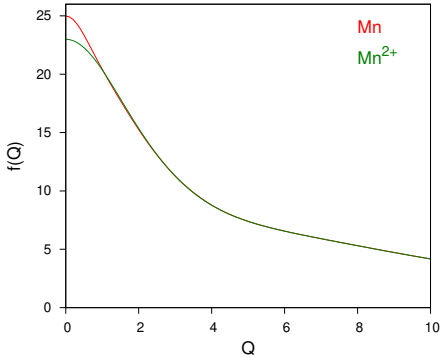
Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

From the *International Tables for Crystallography*



	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Mn	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896
Mn^{2+}	10.8061	5.2796	7.3620	0.3435	3.5268	14.3430	0.2184	41.3235	1.0874

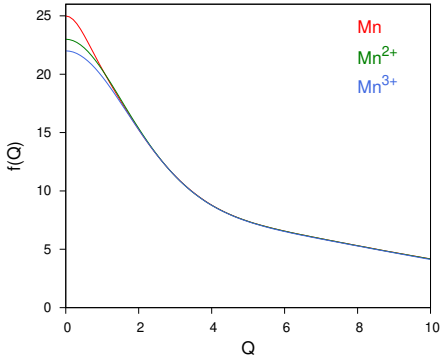
Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

From the *International Tables for Crystallography*



	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Mn	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896
Mn^{2+}	10.8061	5.2796	7.3620	0.3435	3.5268	14.3430	0.2184	41.3235	1.0874
Mn^{3+}	9.8452	4.9180	7.8719	0.2944	3.5653	10.8171	0.3236	24.1281	0.3940

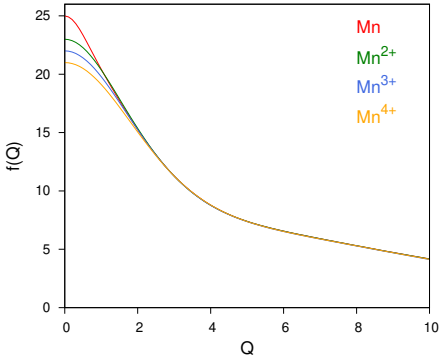
Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

Assuming that this density is spherically symmetric, the form factors are reasonably well approximated by a sum of gaussians

$$f(Q) = \sum_{i=1}^{4} a_i e^{-b_i (Q/2\pi)^2} + c$$

From the *International Tables for Crystallography*



	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Mn	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896
Mn^{2+}	10.8061	5.2796	7.3620	0.3435	3.5268	14.3430	0.2184	41.3235	1.0874
Mn^{3+}	9.8452	4.9180	7.8719	0.2944	3.5653	10.8171	0.3236	24.1281	0.3940
Mn^{4+}	9.9625	4.8485	7.9706	0.2833	2.7607	10.4852	0.0545	27.5730	0.2519

Scattering from molecules

Recall for a single atom we have a form factor

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

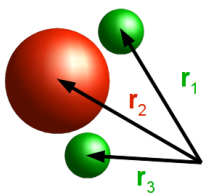
extending to a molecule ...

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...

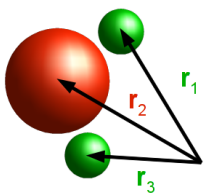


Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...



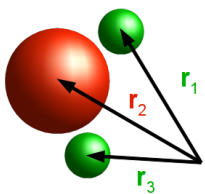
$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...



$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

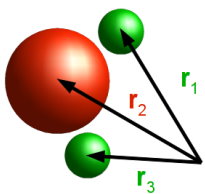
$$F^{molecule}(\mathbf{Q}) =$$

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...



$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

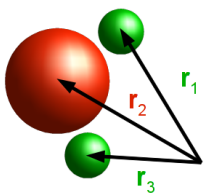
$$F^{molecule}(\mathbf{Q}) = f_1(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_1} +$$

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...



$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

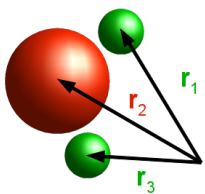
$$F^{molecule}(\mathbf{Q}) = f_1(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_1} + f_2(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_2} +$$

Scattering from molecules

Recall for a single atom we have a form factor

$$f(\mathbf{Q}) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

extending to a molecule ...



$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

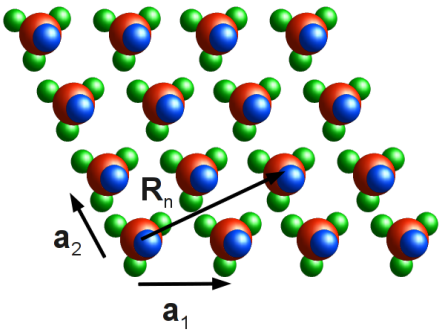
$$F^{molecule}(\mathbf{Q}) = f_1(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_1} + f_2(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_2} + f_3(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_3}$$

Scattering from a crystal

and similarly, to a crystal lattice ...

Scattering from a crystal

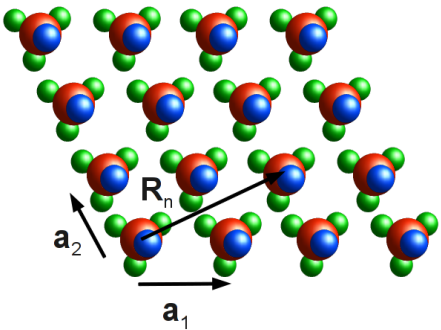
and similarly, to a crystal lattice ...



. . . which is simply a periodic array of molecules

Scattering from a crystal

and similarly, to a crystal lattice ...

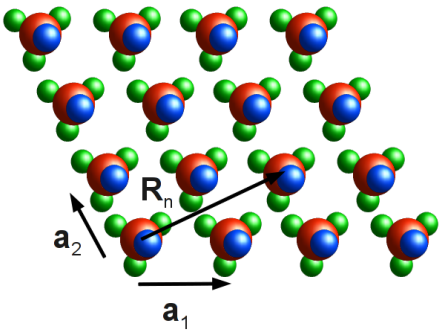


. . . which is simply a periodic array of molecules

$$F^{crystal}(\mathbf{Q}) = F^{molecule} F^{lattice}$$

Scattering from a crystal

and similarly, to a crystal lattice ...



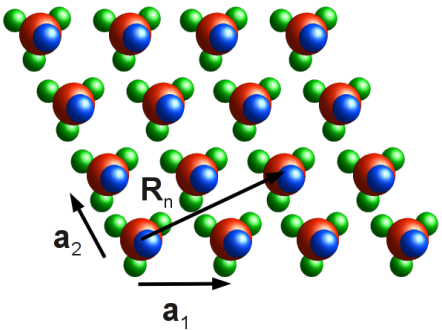
. . . which is simply a periodic array of molecules

$$F^{crystal}(\mathbf{Q}) = F^{molecule} F^{lattice}$$

$$F^{crystal}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j} \sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

Scattering from a crystal

and similarly, to a crystal lattice ...



. . . which is simply a periodic array of molecules

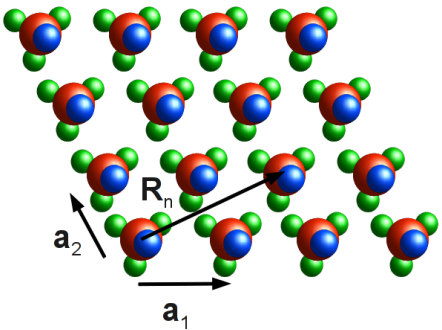
$$F^{crystal}(\mathbf{Q}) = F^{molecule} F^{lattice}$$

$$F^{crystal}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j} \sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

The lattice term, $\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$, is a sum over a large number

Scattering from a crystal

and similarly, to a crystal lattice ...



. . . which is simply a periodic array of molecules

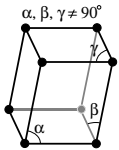
$$F^{crystal}(\mathbf{Q}) = F^{molecule} F^{lattice}$$

$$F^{crystal}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j} \sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

The lattice term, $\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$, is a sum over a large number so it is always small unless $\mathbf{Q}\cdot\mathbf{R}_n = 2\pi m$ where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a real space lattice vector and m is an integer.

Crystal lattices

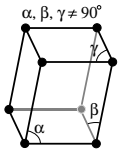
There are 7 possible real space lattices:



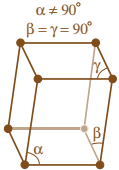
triclinic

Crystal lattices

There are 7 possible real space lattices:



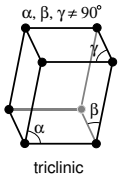
triclinic

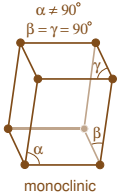


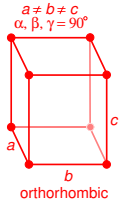
monoclinic

Crystal lattices

There are 7 possible real space lattices:

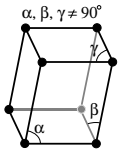




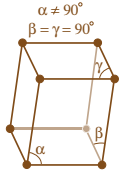


Crystal lattices

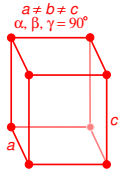
There are 7 possible real space lattices:



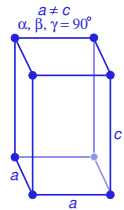
triclinic



monoclinic



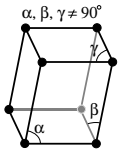
orthorhombic



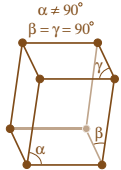
tetragonal

Crystal lattices

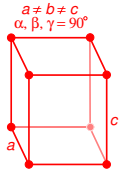
There are 7 possible real space lattices:



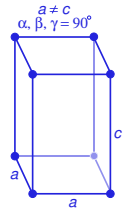
triclinic



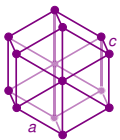
monoclinic



orthorhombic



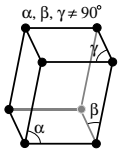
tetragonal



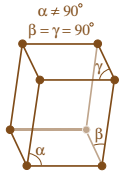
hexagonal

Crystal lattices

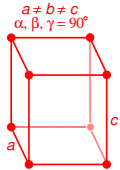
There are 7 possible real space lattices:



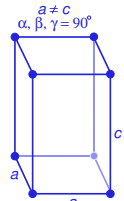
triclinic



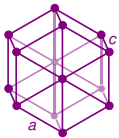
monoclinic



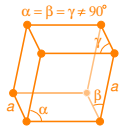
orthorhombic



tetragonal



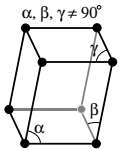
hexagonal



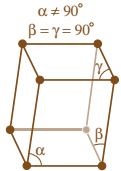
rhombohedral

Crystal lattices

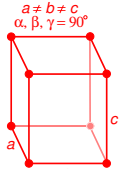
There are 7 possible real space lattices:



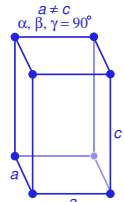
triclinic



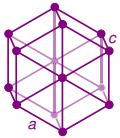
monoclinic



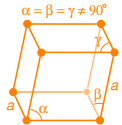
orthorhombic



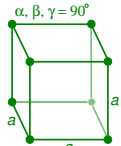
tetragonal



hexagonal



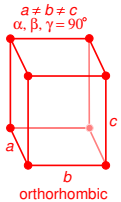
rhombohedral



cubic

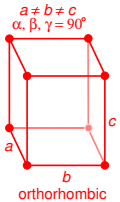
Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



Lattice properties

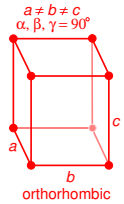
Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).

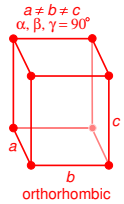


$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



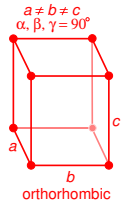
$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$

$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

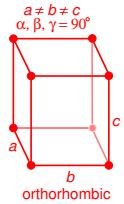
$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$

$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$

$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$

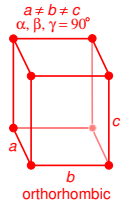
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$

$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

A simple way of calculating the volume of the unit cell!

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$

$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$

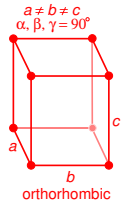
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

A simple way of calculating the volume of the unit cell!

This unit cell is repeated infintely in 3-dimensions and thus, the location of each lattice point can be calculated relative to any arbitrary lattice point designated as the origin.

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$
$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

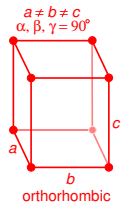
A simple way of calculating the volume of the unit cell!

This unit cell is repeated infintely in 3-dimensions and thus, the location of each lattice point can be calculated relative to any arbitrary lattice point designated as the origin.

Each lattice point is at the end of a lattice vector, $\mathbf{R}_n$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$
$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

A simple way of calculating the volume of the unit cell!

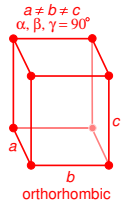
This unit cell is repeated infintely in 3-dimensions and thus, the location of each lattice point can be calculated relative to any arbitrary lattice point designated as the origin.

Each lattice point is at the end of a lattice vector, $\mathbf{R}_n$

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$
$$\mathbf{a}_1 \times \mathbf{a}_2 = ab\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = ab\hat{\mathbf{z}} \cdot c\hat{\mathbf{z}}$$
$$(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = abc = V$$

A simple way of calculating the volume of the unit cell!

This unit cell is repeated infintely in 3-dimensions and thus, the location of each lattice point can be calculated relative to any arbitrary lattice point designated as the origin.

Each lattice point is at the end of a lattice vector, $\mathbf{R}_n$ and a crystal is made by putting a molecule at each lattice point.

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)}$$

$$\mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$

$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}$$

$$\mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$
$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}$$
$$\mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$
$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}$$
$$\mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

$$\mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$
$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}$$
$$\mathbf{a}_3^* = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

$$\mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

where h, k, and l are integers called Miller indices

Laue condition

Because of the construction of the reciprocal lattice

Laue condition

Because of the construction of the reciprocal lattice

$$\mathbf{G}_{hkl} \cdot \mathbf{R}_n$$

Laue condition

Because of the construction of the reciprocal lattice

$$\mathbf{G}_{hkl} \cdot \mathbf{R}_n = (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) \cdot (h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*)$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl} \cdot \mathbf{R}_n &= (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) \cdot (h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*) \\ &= (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) \cdot 2\pi \left(h\frac{\mathbf{a}_2 \times \mathbf{a}_3}{V} + k\frac{\mathbf{a}_3 \times \mathbf{a}_1}{V} + l\frac{\mathbf{a}_1 \times \mathbf{a}_2}{V} \right)\end{aligned}$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor

$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor is non-zero only when

$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}\neq 0$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor is non-zero only when

$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}\neq 0 \qquad\qquad \mathbf{Q}=\mathbf{G}_{hkl}$$

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor is non-zero only when

$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}\neq 0 \qquad\qquad \mathbf{Q}=\mathbf{G}_{hkl}$$

so a significant number of molecules scatter *in phase* with each other

Laue condition

Because of the construction of the reciprocal lattice

$$\begin{aligned}\mathbf{G}_{hkl}\cdot\mathbf{R}_n &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot(h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*)\\ &= (n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3)\cdot 2\pi\left(h\frac{\mathbf{a}_2\times\mathbf{a}_3}{V}+k\frac{\mathbf{a}_3\times\mathbf{a}_1}{V}+l\frac{\mathbf{a}_1\times\mathbf{a}_2}{V}\right)\\ &= 2\pi(hn_1+kn_2+ln_3)=2\pi m\end{aligned}$$

and therefore, the crystal scattering factor is non-zero only when

$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}\neq 0 \qquad\qquad \mathbf{Q}=\mathbf{G}_{hkl}$$

so a significant number of molecules scatter *in phase* with each other

As we shall see later, this Laue condition, is equivalent to the more typically used Bragg condition for diffraction: $2d\sin\theta = n\lambda$

Multiple slit interference

A crystal is, therefore, a diffraction grating with $\sim 10^{20}$ slits!

Multiple slit interference

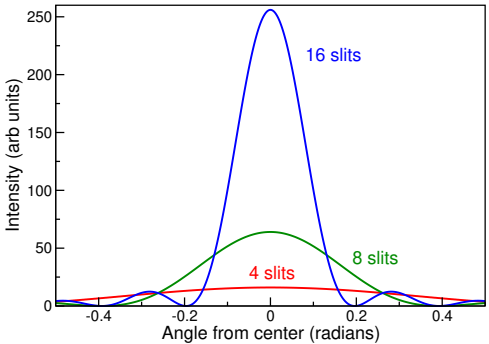
A crystal is, therefore, a diffraction grating with $\sim 10^{20}$ slits!

When $\mathbf{Q}$ is a reciprocal lattice vector, a very strong, narrow diffraction peak is seen at the detector.

Multiple slit interference

A crystal is, therefore, a diffraction grating with $\sim 10^{20}$ slits!

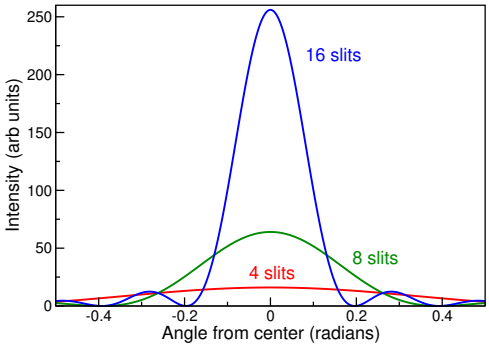
When **Q** is a reciprocal lattice vector, a very strong, narrow diffraction peak is seen at the detector.

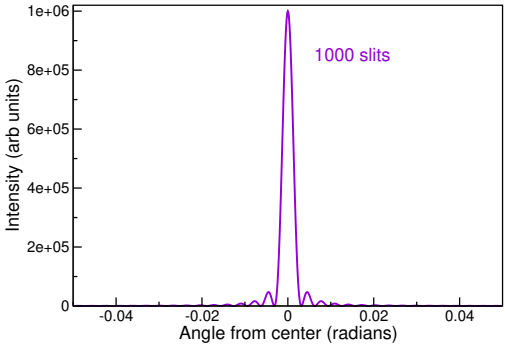


Multiple slit interference

A crystal is, therefore, a diffraction grating with $\sim 10^{20}$ slits!

When **Q** is a reciprocal lattice vector, a very strong, narrow diffraction peak is seen at the detector.



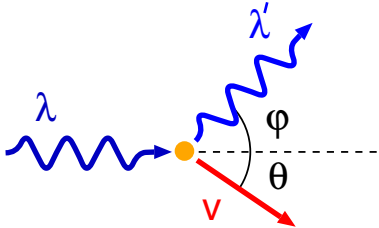


Compton scattering

Consider a photon-electron collision

Compton scattering

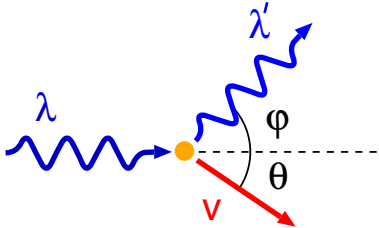
Consider a photon-electron collision



Compton scattering

Consider a photon-electron collision

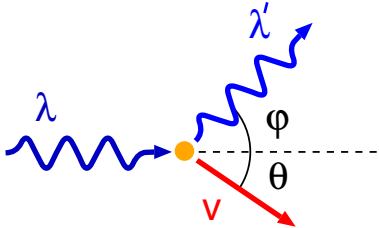
$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$



Compton scattering

Consider a photon-electron collision

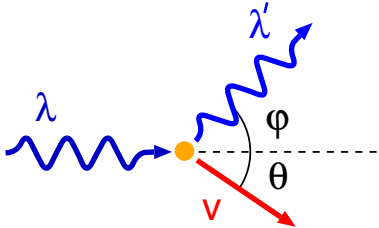
$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$



Compton scattering

Consider a photon-electron collision

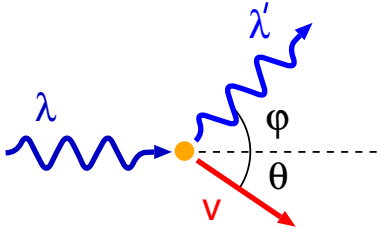
$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$
$$|\mathbf{k}| \neq |\mathbf{k}'|$$



Compton scattering

Consider a photon-electron collision

$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$
$$|\mathbf{k}| \neq |\mathbf{k}'|$$

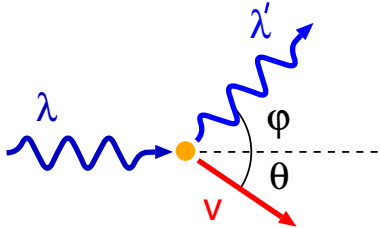


Treat the electron relativistically and conserve energy and momentum

Compton scattering

Consider a photon-electron collision

$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$
$$|\mathbf{k}| \neq |\mathbf{k}'|$$



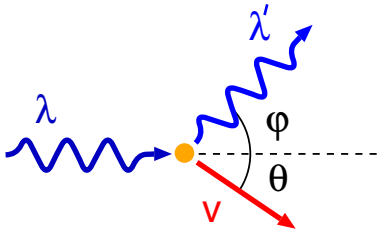
Treat the electron relativistically and conserve energy and momentum

$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \quad \text{(energy)}$$

Compton scattering

Consider a photon-electron collision

$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$
$$|\mathbf{k}| \neq |\mathbf{k}'|$$



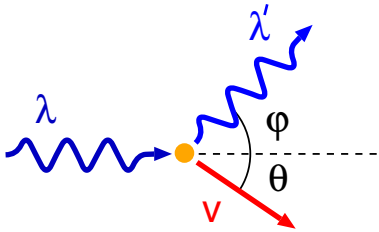
Treat the electron relativistically and conserve energy and momentum

$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \quad \text{(energy)}$$
$$\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma m v \cos\theta \quad \text{(x-axis)}$$

Compton scattering

Consider a photon-electron collision

$$\mathbf{p} = \hbar\mathbf{k} = 2\pi\hbar/\lambda$$
$$\mathbf{p}' = \hbar\mathbf{k}' = 2\pi\hbar/\lambda'$$
$$|\mathbf{k}| \neq |\mathbf{k}'|$$



Treat the electron relativistically and conserve energy and momentum

$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \quad \text{(energy)}$$
$$\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma mv\cos\theta \quad \text{(x-axis)}$$
$$0 = \frac{h}{\lambda'}\sin\phi + \gamma mv\sin\theta \quad \text{(y-axis)}$$

Compton scattering derivation

squaring the momentum equations

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

$$\left(-\frac{h}{\lambda'}\sin\phi\right)^2 = \gamma^2 m^2 v^2 \sin^2\theta$$

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

$$\left(-\frac{h}{\lambda'}\sin\phi\right)^2 = \gamma^2 m^2 v^2 \sin^2\theta$$

now add them together,

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

$$\left(-\frac{h}{\lambda'}\sin\phi\right)^2 = \gamma^2 m^2 v^2 \sin^2\theta$$

now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares,

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

$$\gamma^2 m^2 v^2 = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}\sin^2\phi + \frac{h^2}{\lambda'^2}\cos^2\phi$$

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

$$\left(-\frac{h}{\lambda'}\sin\phi\right)^2 = \gamma^2 m^2 v^2 \sin^2\theta$$

now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares, and $\sin^2\phi + \cos^2\phi = 1$, then rearrange

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

$$\gamma^2 m^2 v^2 = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}\sin^2\phi + \frac{h^2}{\lambda'^2}\cos^2\phi$$

$$\frac{m^2 v^2}{1-\beta^2} = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}$$

Compton scattering derivation

squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

$$\left(-\frac{h}{\lambda'}\sin\phi\right)^2 = \gamma^2 m^2 v^2 \sin^2\theta$$

now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares, and $\sin^2\phi + \cos^2\phi = 1$, then rearrange and substitute $v = \beta c$

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

$$\gamma^2 m^2 v^2 = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}\sin^2\phi + \frac{h^2}{\lambda'^2}\cos^2\phi$$

$$\frac{m^2 c^2 \beta^2}{1-\beta^2} = \frac{m^2 v^2}{1-\beta^2} = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it,

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it, then solve it for β^2

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

$$\beta^2 = 1 - \frac{m^2 c^4}{\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it, then solve it for β^2 which is substituted into the equation from the momentum.

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

$$\beta^2 = 1 - \frac{m^2 c^4}{\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2}$$

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \frac{m^2 c^2 \beta^2}{1-\beta^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it, then solve it for β^2 which is substituted into the equation from the momentum.

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

$$\beta^2 = 1 - \frac{m^2 c^4}{\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2}$$

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \frac{m^2 c^2 \beta^2}{1-\beta^2}$$

$$= \frac{1}{c^2}\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 - m^2 c^2$$

Compton scattering derivation (cont.)

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

Compton scattering derivation (cont.)

After expansion,

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

$$= m^2c^2 + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - m^2c^2$$

Compton scattering derivation (cont.)

After expansion, cancellation,

$$\begin{aligned}\frac{h^2}{\lambda^2}+\frac{h^2}{\lambda'^2}-\frac{2h^2}{\lambda\lambda'}\cos\phi &= \left(mc+\frac{h}{\lambda}-\frac{h}{\lambda'}\right)^2 - m^2c^2 \\ &= \cancel{m^2c^2}+\frac{h^2}{\lambda^2}+\frac{h^2}{\lambda'^2}-\frac{2mch}{\lambda}-\frac{2mch}{\lambda'}+\frac{2h^2}{\lambda\lambda'}-\cancel{m^2c^2} \\ &= 2m\left(\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)+\frac{h^2}{\lambda^2}+\frac{h^2}{\lambda'^2}-\frac{2h^2}{\lambda\lambda'}\end{aligned}$$

Compton scattering derivation (cont.)

After expansion, cancellation,

$$\begin{aligned}\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi &= \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2 \\ &= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2} \\ &= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\end{aligned}$$

Compton scattering derivation (cont.)

After expansion, cancellation, and rearrangement, we obtain

$$\begin{aligned}\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi &= \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2 \\ &= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2} \\ &= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\end{aligned}$$

$$\frac{2h^2}{\lambda\lambda'}(1 - \cos\phi) = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)$$

Compton scattering derivation (cont.)

After expansion, cancellation,

$$\begin{aligned}\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi &= \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2 \\ &= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2} \\ &= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\end{aligned}$$

$$\frac{2h^2}{\lambda\lambda'}(1 - \cos\phi) = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) = 2mhc\left(\frac{\lambda' - \lambda}{\lambda\lambda'}\right)$$

Compton scattering derivation (cont.)

After expansion, cancellation,

$$\begin{aligned}\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi &= \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2 \\ &= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2} \\ &= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\end{aligned}$$

$$\frac{2h^2}{\lambda\lambda'}(1-\cos\phi) = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) = 2mhc\left(\frac{\lambda'-\lambda}{\lambda\lambda'}\right) = \frac{2mhc\Delta\lambda}{\lambda\lambda'}$$

Compton scattering derivation (cont.)

After expansion, cancellation,

$$\frac{\cancel{h^2}}{\cancel{\lambda^2}} + \frac{\cancel{h^2}}{\cancel{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

$$= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2}$$

$$= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \frac{\cancel{h^2}}{\cancel{\lambda^2}} + \frac{\cancel{h^2}}{\cancel{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}$$

$$\frac{2h^2}{\cancel{\lambda\lambda'}}(1 - \cos\phi) = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) = 2mhc\left(\frac{\lambda' - \lambda}{\lambda\lambda'}\right) = \frac{2mhc\Delta\lambda}{\cancel{\lambda\lambda'}}$$

$$\Delta\lambda = \frac{h}{mc}(1 - \cos\phi)$$

Compton scattering results

Thus, for an electron

Compton scattering results

Thus, for an electron

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å}$$

Compton scattering results

Thus, for an electron

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å}$$

$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-5}\text{Å}$$

Compton scattering results

Thus, for an electron

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å}$$
$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-5}\text{Å}$$

Comparing the two scattering lengths:

$$r_0/\lambda_C = 1/137$$

Compton scattering results

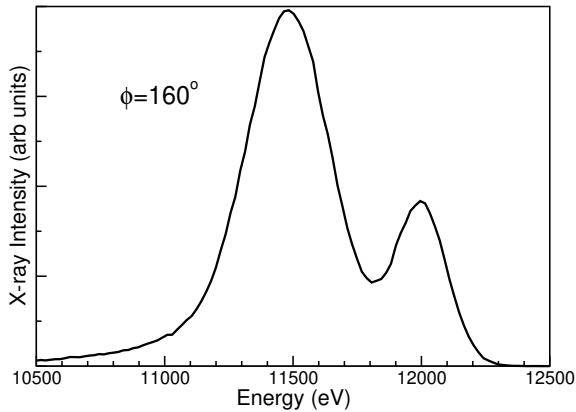
Thus, for an electron

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å}$$

$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-5}\text{Å}$$

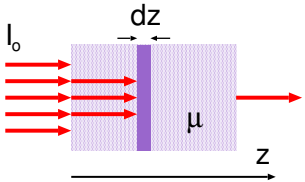
Comparing the two scattering lengths:

$$r_0/\lambda_C = 1/137$$

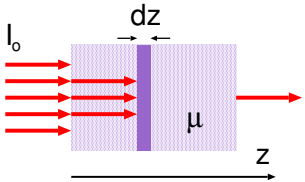


Scattering of 12 keV x-rays from a silicon wafer at 160° with a bent crystal wavelength dispersive analyzer

X-ray absorption

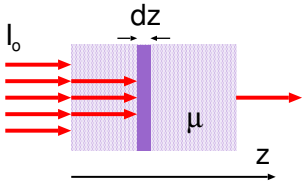


X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

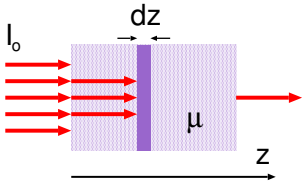
X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz$$

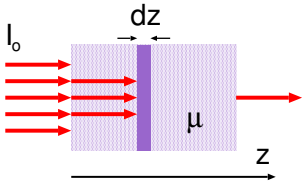
X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

X-ray absorption

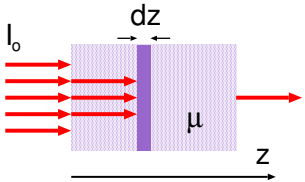


For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

integrating both sides

X-ray absorption



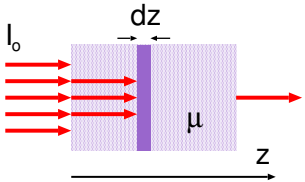
For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz$$

integrating both sides

X-ray absorption



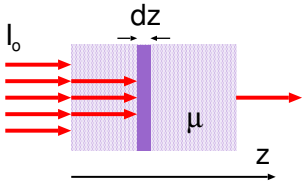
For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

integrating both sides

X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

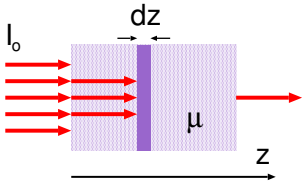
$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

integrating both sides

and taking the anti-log

X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

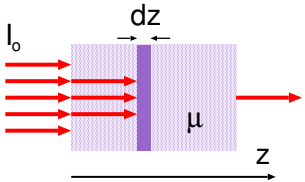
$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

integrating both sides

and taking the anti-log

$$I = e^{C} e^{-\mu z} = Ae^{-\mu z}$$

X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

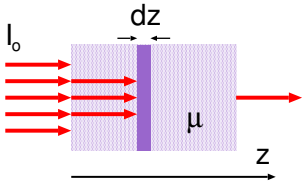
integrating both sides

$$I = e^C e^{-\mu z} = Ae^{-\mu z}$$

and taking the anti-log

if the intensity at $z = 0$ is I_0, then

X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

integrating both sides

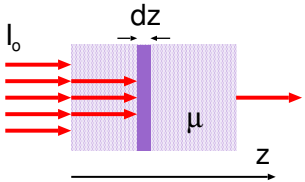
$$I = e^{C} e^{-\mu z} = A e^{-\mu z}$$

and taking the anti-log

$$I = I_0 e^{-\mu z}$$

if the intensity at $z = 0$ is I_0, then

X-ray absorption



For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

$$dI = -I(z)\mu dz \longrightarrow \frac{dI}{I(z)} = -\mu dz$$

$$\int \frac{dI}{I(z)} = -\int \mu dz \longrightarrow \ln(I) = -\mu z + C$$

integrating both sides

$$I = e^C e^{-\mu z} = Ae^{-\mu z}$$

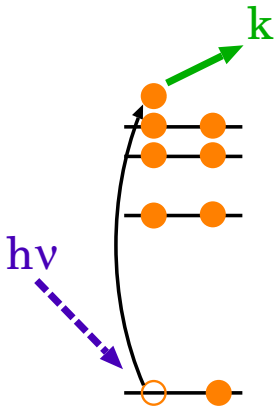
and taking the anti-log

$$I = I_0 e^{-\mu z}$$

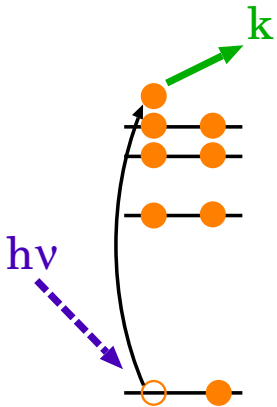
if the intensity at $z = 0$ is I_0, then

This is just Beer's law with an absorption coefficient which depends on x-ray parameters.

Absorption event

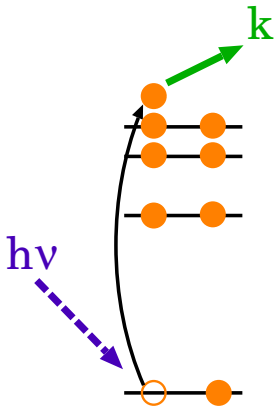


Absorption event



X-ray is absorbed by an atom

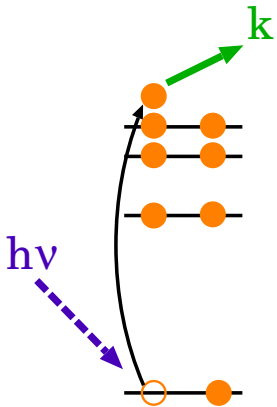
Absorption event



X-ray is absorbed by an atom

Energy is transferred to a core electron

Absorption event

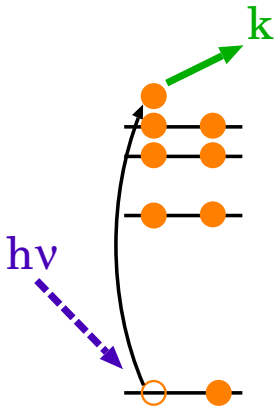


X-ray is absorbed by an atom

Energy is transferred to a core electron

Electron escapes atomic potential into the continuum

Absorption event



X-ray is absorbed by an atom

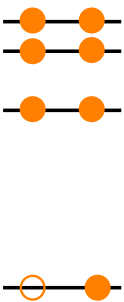
Energy is transferred to a core electron

Electron escapes atomic potential into the continuum

Ion remains with a core-hole

Fluorescence emission

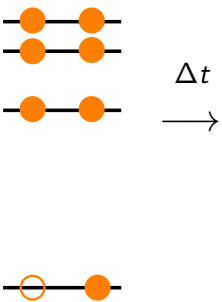
An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)



Fluorescence emission

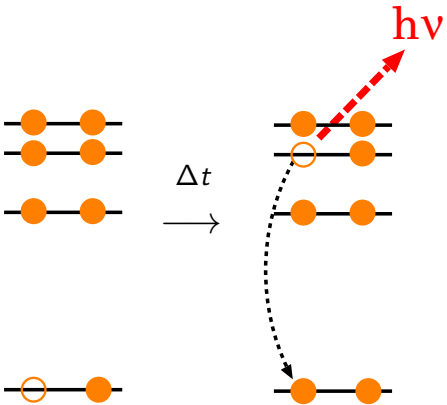
An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)

After a short time a higher level electron will drop down in energy to fill the core hole



Fluorescence emission

An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)

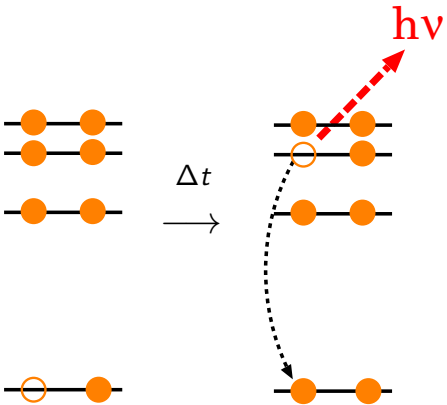


After a short time a higher level electron will drop down in energy to fill the core hole

Energy is liberated in the form of a fluorescence photon

Fluorescence emission

An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)



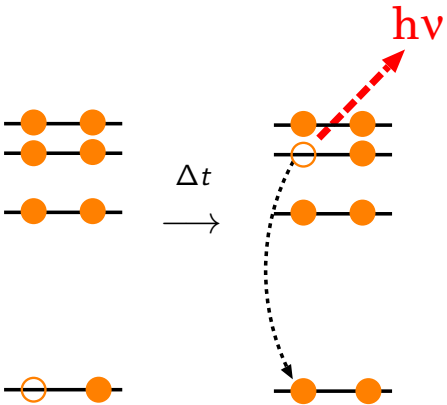
After a short time a higher level electron will drop down in energy to fill the core hole

Energy is liberated in the form of a fluorescence photon

This leaves a second hole (not core) which is then filled from an even higher shell

Fluorescence emission

An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)



After a short time a higher level electron will drop down in energy to fill the core hole

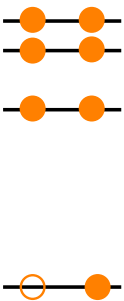
Energy is liberated in the form of a fluorescence photon

This leaves a second hole (not core) which is then filled from an even higher shell

The result is a cascade of fluorescence photons which are characteristic of the absorbing atom

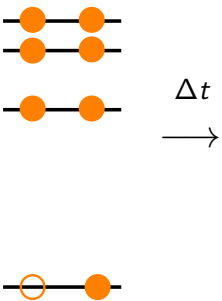
Auger emission

While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms



Auger emission

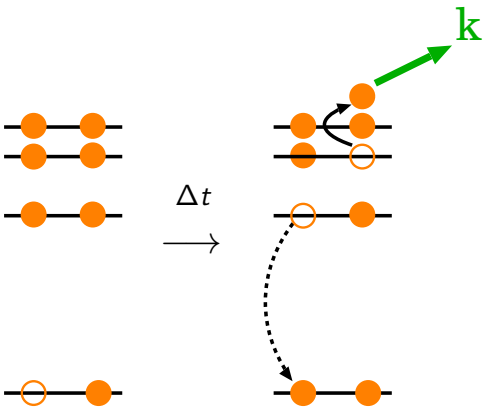
While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms



In the Auger process, a higher level electron will drop down in energy to fill the core hole

Auger emission

While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms

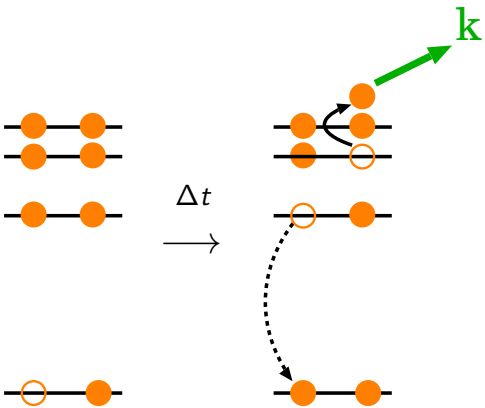


In the Auger process, a higher level electron will drop down in energy to fill the core hole

The energy liberated causes the secondary emission of an electron

Auger emission

While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms



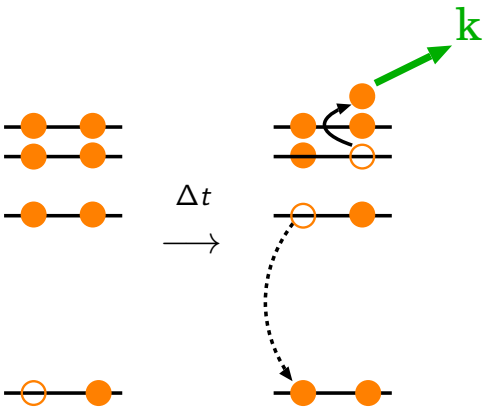
In the Auger process, a higher level electron will drop down in energy to fill the core hole

The energy liberated causes the secondary emission of an electron

This leaves two holes which then filled from higher shells

Auger emission

While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms



In the Auger process, a higher level electron will drop down in energy to fill the core hole

The energy liberated causes the secondary emission of an electron

This leaves two holes which then filled from higher shells

So that the secondary electron is accompanied by fluorescence emissions at lower energies

Absorption coefficient

The absorption coefficient μ,

$$\mu \sim \text{——}$$

Absorption coefficient

The absorption coefficient μ, depends strongly on the x-ray energy E,

$$\mu \sim \frac{}{E^3}$$

Absorption coefficient

The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z,

$$\mu \sim \frac{Z^4}{E^3}$$

Absorption coefficient

The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z, as well as the density ρ,

$$\mu \sim \frac{\rho Z^4}{E^3}$$

Absorption coefficient

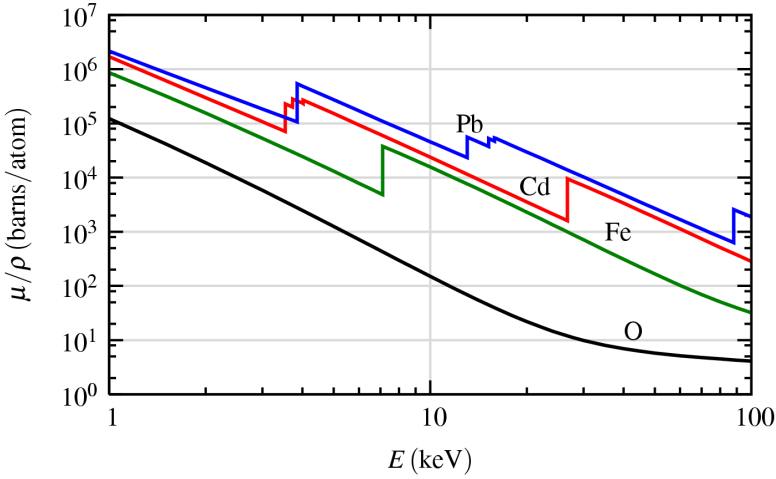
The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z, as well as the density ρ, and atomic mass A:

$$\mu \sim \frac{\rho Z^4}{A E^3}$$

Absorption coefficient

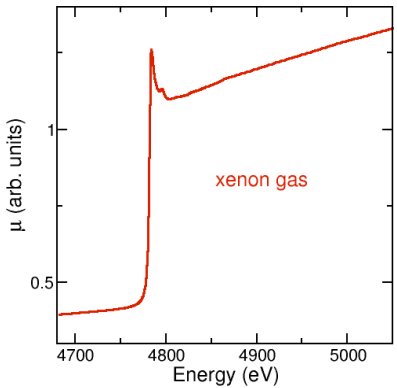
The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z, as well as the density ρ, and atomic mass A:

$$\mu \sim \frac{\rho Z^4}{A E^3}$$



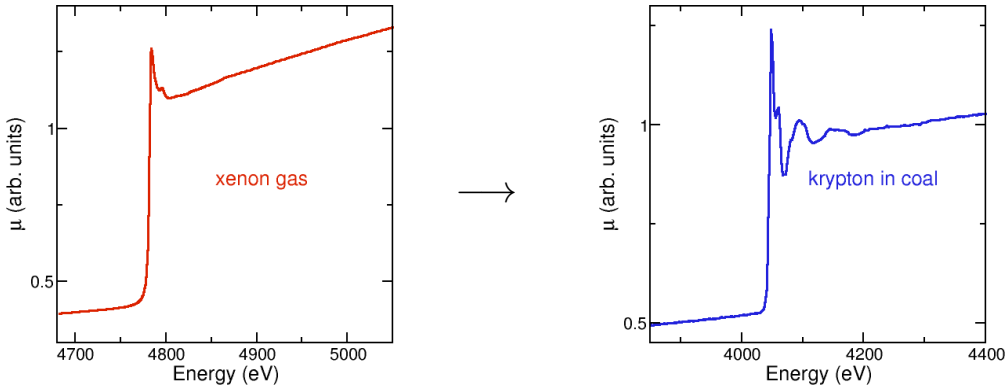
Absorption coefficient

Isolated gas atoms show a sharp jump and a smooth curve



Absorption coefficient

Isolated gas atoms show a sharp jump and a smooth curve but atoms in a solid or liquid show fine structure after the absorption edge called XANES and EXAFS



Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

$$\mu = \rho_a \sigma_a$$

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

rewriting in terms of the mass density, ρ_m, the atomic mass, M_a, and Avogadro's number, N_A, the absorption coefficient becomes

$$\mu = \rho_a \sigma_a$$

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

rewriting in terms of the mass density, ρ_m, the atomic mass, M_a, and Avogadro's number, N_A, the absorption coefficient becomes

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{M_a} \right) \sigma_a$$

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

rewriting in terms of the mass density, ρ_m, the atomic mass, M_a, and Avogadro's number, N_A, the absorption coefficient becomes

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{M_a} \right) \sigma_a$$

if the absorber is made up of a number of different atoms, this calculation can be generalized

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

rewriting in terms of the mass density, ρ_m, the atomic mass, M_a, and Avogadro's number, N_A, the absorption coefficient becomes

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{M_a} \right) \sigma_a$$

if the absorber is made up of a number of different atoms, this calculation can be generalized

$$\mu = \sum_j \rho_j \sigma_{aj}$$

Absorption calculations

For an elemental material, the absorption coefficient, μ, is simply the product of the atomic density, ρ_a, times the atomic absorption cross-section, σ_a.

rewriting in terms of the mass density, ρ_m, the atomic mass, M_a, and Avogadro's number, N_A, the absorption coefficient becomes

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{M_a} \right) \sigma_a$$

if the absorber is made up of a number of different atoms, this calculation can be generalized

$$\mu = \sum_j \rho_j \sigma_{aj}$$

where ρ_j and σ_{aj} are the atomic density and atomic absorption cross-section of each component

Absorption coefficient of a compound

$\mu[\mathrm{cm}^{-}1]$ is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, $\mu_m[\mathrm{cm}^2/\mathrm{g}]$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

$$\mu_m = (N_A/M_c) \sum_j x_j \sigma_{aj}$$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

$$\mu_m = (N_A/M_c) \sum_j x_j \sigma_{aj}$$

The "thickness" of a mass m of the compound, distributed over an area A is then:

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

$$\mu_m = (N_A/M_c) \sum_j x_j \sigma_{aj}$$

The "thickness" of a mass m of the compound, distributed over an area A is then:

$$z = \frac{m}{\rho_c A}$$

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

$$\mu_m = (N_A/M_c) \sum_j x_j \sigma_{aj}$$

The "thickness" of a mass m of the compound, distributed over an area A is then:

$$z = \frac{m}{\rho_c A}$$

This leads to an absorption per unit mass of μ_m/A and Beer's law becomes

Absorption coefficient of a compound

μ[cm$^-$1] is the linear absorption coefficient. It is useful in practice to define the mass absorption coefficient, μ_m[cm^2/g]

$$\mu_m = \mu/\rho$$

Beer's Law now becomes

$$I = I_0 e^{-\mu z} = I_0 e^{-\mu_m \rho z}$$

Suppose we want to compute the absorption coefficient per unit mass of a compound if we distribute it over an area A

If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

$$M_c = \sum_j x_j M_j$$

$$\mu_m = (N_A/M_c) \sum_j x_j \sigma_{aj}$$

The "thickness" of a mass m of the compound, distributed over an area A is then:

$$z = \frac{m}{\rho_c A}$$

This leads to an absorption per unit mass of μ_m/A and Beer's law becomes

$$I = I_0 e^{-(\mu_m/A)m}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A \sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m}, \ \mu_m = \frac{N_A}{M_c} \sum_j x_j \sigma_{aj}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j\sigma_j$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j\sigma_j$$

the molecular mass and density of Fe_2O_3 are

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j\sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j\sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j\sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

$$M_{Fe} = 55.895\,\mathrm{g/mol}$$

$$M_O = 16.000\,\mathrm{g/mol}$$

assuming a 5 mm diameter pellet

$$M_c = 159.69\,\mathrm{g/mol}$$

$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$

$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$
$$A = \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$
$$A = \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

$$\mu_m = \frac{1}{159.69}\left[2\cdot 55.895\cdot 138.860 + 3\cdot 16.000\cdot 46.666\right]$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$
$$A = \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

$$\mu_m = \frac{1}{159.69}\left[2\cdot 55.895\cdot 138.860 + 3\cdot 16.000\cdot 46.666\right] = 111.23\,\mathrm{cm^2/g}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$
$$A = \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

$$\mu_m = \frac{1}{159.69}\left[2\cdot 55.895\cdot 138.860 + 3\cdot 16.000\cdot 46.666\right]$$
$$= 111.23\,\mathrm{cm^2/g} \quad\longrightarrow\quad \mu_\mathrm{m}/\mathrm{A} = 566.7\,\mathrm{g^{-1}}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

$$\begin{aligned}
\rho &= 5.24\,\mathrm{g/cm^3}\\
M_{Fe} &= 55.895\,\mathrm{g/mol}\\
M_O &= 16.000\,\mathrm{g/mol}\\
M_c &= 159.69\,\mathrm{g/mol}\\
\sigma_{Fe} &= 138.860\,\mathrm{cm^2/g}\\
\sigma_O &= 46.666\,\mathrm{cm^2/g}\\
A &= \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}
\end{aligned}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

$$\begin{aligned}
\mu_m &= \frac{1}{159.69}\left[2\cdot 55.895\cdot 138.860 + 3\cdot 16.000\cdot 46.666\right]\\
&= 111.23\,\mathrm{cm^2/g} \quad\longrightarrow\quad \mu_\mathrm{m}/\mathrm{A} = 566.7\,\mathrm{g^{-1}}\\
\mu &= \mu_m\rho = 582.9\,\mathrm{cm^{-1}},
\end{aligned}$$

Absorption of Fe_2O_3 at 5 keV

The most commonly tabulated cross-sections are not the atomic cross-sections but the mass cross sections, $\sigma_j = N_A\sigma_{aj}/M_j$ so we have

$$I = I_0 e^{-(\mu_m/A)m},\ \mu_m = \frac{N_A}{M_c}\sum_j x_j\sigma_{aj} = \frac{N_A}{M_c}\sum_j \frac{M_j}{N_A}x_j\sigma_j = \frac{1}{M_c}\sum_j M_j x_j \sigma_j$$

the molecular mass and density of Fe_2O_3 are

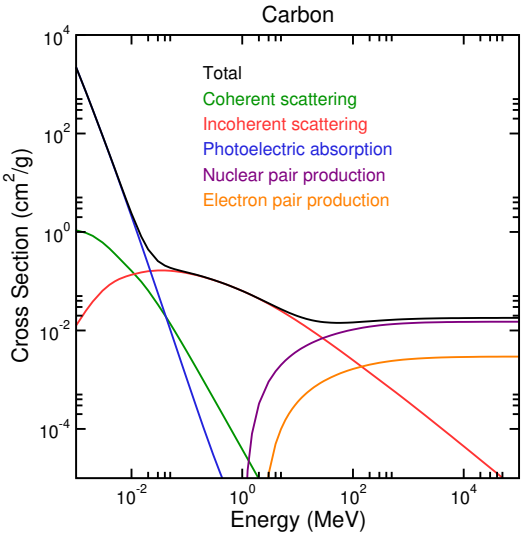
$$\rho = 5.24\,\mathrm{g/cm^3}$$
$$M_{Fe} = 55.895\,\mathrm{g/mol}$$
$$M_O = 16.000\,\mathrm{g/mol}$$
$$M_c = 159.69\,\mathrm{g/mol}$$
$$\sigma_{Fe} = 138.860\,\mathrm{cm^2/g}$$
$$\sigma_O = 46.666\,\mathrm{cm^2/g}$$
$$A = \pi(0.25\,\mathrm{cm})^2 = 0.1963\,\mathrm{cm^2}$$

begin by finding tabulated values of the cross-section for the elements Fe and O at 5 keV

assuming a 5 mm diameter pellet

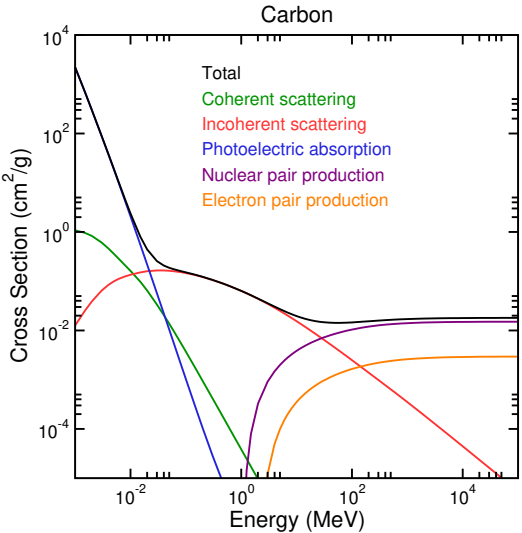
$$\mu_m = \frac{1}{159.69}\left[2\cdot 55.895\cdot 138.860 + 3\cdot 16.000\cdot 46.666\right]$$
$$= 111.23\,\mathrm{cm^2/g} \quad\longrightarrow\quad \mu_m/\mathrm{A} = 566.7\,\mathrm{g^{-1}}$$
$$\mu = \mu_m\rho = 582.9\,\mathrm{cm^{-1}}, \quad\longrightarrow\quad 1/\mu = 17.2\,\mu\mathrm{m}$$

Comparison of cross sections



Comparison of cross sections

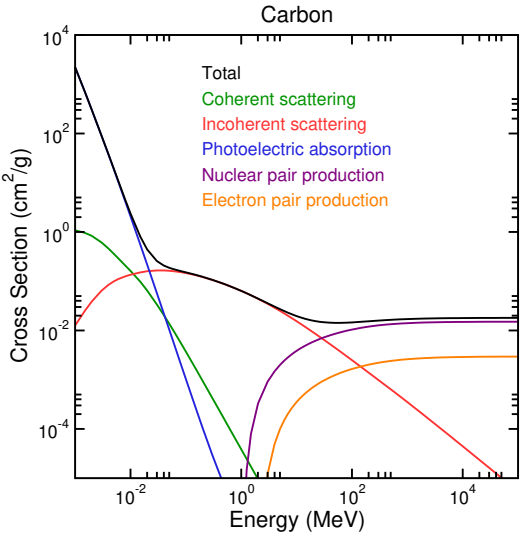
Photoelectric absorption dominates at low energies



Comparison of cross sections

Photoelectric absorption dominates at low energies

Thomson scattering (coherent) drops rapidly with energy

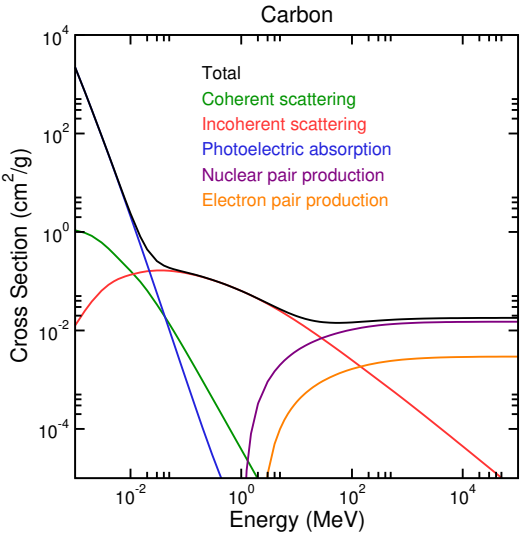


Comparison of cross sections

Photoelectric absorption dominates at low energies

Thomson scattering (coherent) drops rapidly with energy

Compton scattering (incoherent) dominates at medium energies



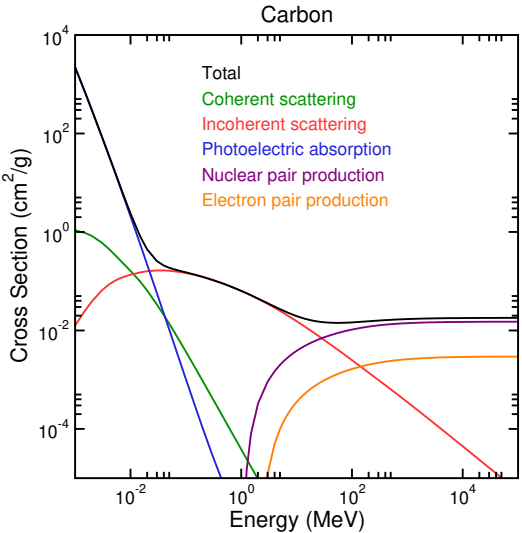
Comparison of cross sections

Photoelectric absorption dominates at low energies

Thomson scattering (coherent) drops rapidly with energy

Compton scattering (incoherent) dominates at medium energies

Pair production dominates at high energies



Comparison of cross sections

Photoelectric absorption dominates at low energies

Thomson scattering (coherent) drops rapidly with energy

Compton scattering (incoherent) dominates at medium energies

Pair production dominates at high energies

Each portion of the cross-section is element-dependent