Crystallography and X-ray diffraction
Characteristics and generation of X-ray
Visible light (~4000 to ~7000 Å)

Visible Light Region of the Electromagnetic Spectrum

Infrared

UltraViolet
Nature of X-ray

<table>
<thead>
<tr>
<th>Wavelength (Angstroms)</th>
<th>Wavelength (centimeters)</th>
<th>Frequency (Hz)</th>
<th>Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 - 0.1</td>
<td>10^{-7} - 10^{-9}</td>
<td>3 \times 10^{17} - 3 \times 10^{19}</td>
<td>10^{3} - 10^{5}</td>
</tr>
</tbody>
</table>

\[ \nu = \frac{c}{\lambda} \quad E = h \nu \]

\( E \) is the energy of the X-ray in keV
\( h \) is Planck’s constant (4.135 \times 10^{-15} \text{ eV} \text{s})
\( c \) is the speed of light (3 \times 10^{18} \text{ Å/s})
\( \lambda \) is the wavelength in Å
\( \nu \) is the photon frequency
For visible lights

(index of refraction)
Index of refraction of x-rays

\[ n = 1 - \alpha + i\beta \]

\[ \alpha = \frac{r_e \lambda^2 Z}{2\pi m_n A_{\text{eff}}} \rho \]

- \( r_e \): the classical electron radius (2.82x10^{-15} \text{m})
- \( \lambda \): the x-ray wavelength
- \( m_n \): the nucleon mass (1.66x10^{-27} \text{kg})
- \( Z/A_{\text{eff}} \): the \( Z \) (atomic number) to \( A \) (atomic mass number) ratio for the material (\( \sim 0.5 \))
- \( \rho \): the mass density of the material

\[ \alpha \sim 10^{-6} \quad => \quad n \sim 1 \]
For X-rays

(n_1 n_2 n_1) (index of refraction)
X-ray is electromagnetic radiation

=> X-ray can be scattered as a wave
Generation of X-ray

- Atom’s characteristic x-ray emission
- Charge particle acceleration / deceleration
Atomic characteristic x-ray emission

Electron energy shells in an atom:
Conventional X-ray tube for X-ray production

Coupling to a high voltage cable

Cathode

X-rays

Be window

Anode

X-rays

Water

Be windows

Water in
Location of X-ray windows for line focus and point focus
Spectrum of X-rays from a conventional X-ray tube

Source of intense peaks (Characteristic lines): electron’s transition from L to K shell (Kα), M to K shell (Kβ).

Source of continuous spectrum (Bramsstrahlung): rapid electron deceleration
Characteristic wavelengths of five common anode materials and the K absorption edges of suitable β-filter materials.¹

<table>
<thead>
<tr>
<th>Metal</th>
<th>Wavelength (Å)</th>
<th>β filter</th>
<th>K-absorption edge, (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$K_\alpha^a$</td>
<td>$K_\alpha_1$</td>
<td>$K_\alpha_2$</td>
</tr>
<tr>
<td>Cr</td>
<td>2.29105</td>
<td>2.28975(3)</td>
<td>2.293652(2)</td>
</tr>
<tr>
<td>Fe</td>
<td>1.93739</td>
<td>1.93608(1)</td>
<td>1.94002(1)</td>
</tr>
<tr>
<td>Co</td>
<td>1.79030</td>
<td>1.7900(1)</td>
<td>1.79289(1)</td>
</tr>
<tr>
<td>Cu</td>
<td>1.54187</td>
<td>1.5405929(5)</td>
<td>1.54441(2)</td>
</tr>
<tr>
<td>Mo</td>
<td>0.71075</td>
<td>0.7093171(4)</td>
<td>0.71361(1)</td>
</tr>
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<td></td>
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</tbody>
</table>

a The weighted average value, calculated as $\lambda_{average} = (2\lambda_{K\alpha_1} + \lambda_{K\alpha_2})/3$. 
\[ \lambda(K\alpha_{\text{ave}}) = \frac{2 \cdot (\lambda(K\alpha_1) + \lambda(K\alpha_2))}{3} \]

The intensity of the \( K\alpha \)

\[ I_k = B \cdot i \cdot (V - V_k)^{1.5} \]

\( i \): applied current

\( V_k \): excitation potential of the target material

\( V \): applied voltage
Compute $\lambda_{SW}$ of the “white” spectrum

Electron kinetic energy: $\frac{1}{2}mv^2 = eV$
- $m$: electron mass
- $v$: velocity
- $e$: the charge of electron (1.602x10^{-19} Coulomb)

Photon energy: $h\nu = \frac{hc}{\lambda}$
- $h$: Planck’s constant (6.626x10^{-34} J•s)
- $\nu$: photon frequency
- $c$: the speed of light in vacuum
- $\lambda$: photon wavelength

Duane-Hunt limit, $(eV = h\frac{c}{\lambda})$

$$\lambda_{SW} = \frac{hc}{eV} = 12.398/V$$
($(V$ in kV, $\lambda_{SW}$ in Å))
The integrated intensity of the “white” spectrum

\[ I_w = A \, i \, Z \, V^n, \quad n \sim 2 \]

i is the applied current
Z is the atomic number of the target
V is the applied voltage
A is a proportionality constant.

Increasing X-ray output of an X-ray tube:

\[ I_k = B \, i \, (V - V_k)^{1.5} \]

\[ \frac{I_k}{I_w} = B \, (V - V_k)^{1.5} / A \, Z \, V^2 \]

**Homework:**
What is the relation between applied voltage (V) and the excitation potential of the target material (V_k) to maximize \( \frac{I_k}{I_w} \)
Homework is due on 10/24